Improving crop models with respect to yield variability and climate extremes as a precondition for food security assessments

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Abstract

Agriculture is a cornerstone of food security, producing eighty percent of the calories that we consume either directly as food or indirectly as animal feed. Production increases in agriculture have contributed to achieve food security for the large majority of people in recent decades, with 'food security' defined as a situation where all people at all times have nutritious and sufficient food. Nevertheless, there are still more than one billion people who are malnourished, and multiple threats are looming for the future of food security. A growing population and dietary shifts towards more animal-based food will increase the demand for agricultural production. At the same time, production capacity is under pressure, in particular by climate change. Even though the impact of climate change is uncertain, climate variability and extremes are likely to increase with it and may diminish harvests. Hence it is decisive to quantify the influences of climate on production. An important tool to quantify climatic influences on crop yields are crop models, which are mathematical descriptions of plant growth and yield. These crop models have matured over decades, but deficiencies remain. Therefore this thesis aims at improving crop models by addressing deficiencies with respect to yield variability and climate extremes. It consists of four parts.

The first part is a meta-study, presenting a new appraisal and structurization of the abundant literature knowledge on crop physiology. A novel method is used to build a network-based encyclopedia, which enables a consistent and systematic classification of diverse physiological influences on crop growth. The network then allows for deducing improvement suggestions for crop models. Two of these suggestions, namely crop damage from ozone pollution and extreme temperatures, are treated in the remaining chapters.

The second part presents a study of ozone damages on historical crop yields. A newly developed ozone module is implemented in the global crop model LPJmL. The enhanced model is used to simulate global historical wheat and soybean yield losses from ozone pollution. Crop water status, temperature and CO_2 are considered as modulators of ozone damage, which constitutes an improvement over previous global assessments that were based on linear correlations between ozone and yield. The analysis indicates that ozone is a major problem for crop production, causing yield losses up to occasional 50%.

The third part contains an analysis of the effects of high temperatures on yield losses in the US, a major crop producing country. Heat waves are likely to occur more frequently under global warming, which requires crop models to correctly simulate their effects on crop yields. Yet it has recently been doubted whether current models are capable of doing so. Hence it is assessed to what extent nine state-of-the-art crop models can reproduce observed effects of high temperatures on maize, soybean and wheat yields in the US. The analysis reveals that the ensemble of crop models reproduces observed yield losses in the correct quantities. The novel combination of statistical and process-based crop models applied here allows for new mechanistic insights, suggesting that yield losses stem from water stress rather than direct heat damages. This justifies irrigation as an effective adaptation measure, at least until a temperature threshold of approx. 36°C where sufficient observations are available. Furthermore, it is hypothesized that future US yields are likely to suffer from heat losses even under elevated CO_2. This is contrary to current convictions and deserves further investigation in experiments.

The fourth part describes a statistical model to assess the global share of weather-driven yield variability and the influence of individual weather variables during different phenological phases. It is decisive to know these influences for designing yield insurances and projecting future yields. An existing statistical model is enhanced by penalties for hot and cold temperature stress, as suggested by the meta-study in part one. With the enhanced model the influence of weather on yield variability of maize, wheat and soybeans is quantified as 15-42% globally, with magnitude and robustness depending on crop and yield input data quality. The model can also be applied for near-term yield forecasting during the growing season. Such pre-harvest knowledge of expected yields is important for management planning at the farm and regional level. First results with a forecasting capacity of more than 50% two months before harvest in several countries merit further development.

Taken together, this thesis underlines the negative influence of ozone and high temperature stress on agricultural production and, consequently, food security. Different crop models are utilized and improved and the benefits of using diverse types of models are highlighted. Perspectives for further research on ozone, extreme heat stress and yield forecasting are presented.

Zusammenfassung

Die Landwirtschaft liefert einen fundamentalen Beitrag zur Ernährungssicherheit, indem sie 80% der vom Menschen verzehrten Kalorien bereitstellt, sowohl als menschliche Nahrung als auch als Futtermittel. Produktionszuwächse in den letzten Jahrzehnten haben dazu beigetragen, Ernährungssicherheit für die große Mehrheit der Bevölkerung zu erreichen. Dabei ist Ernährungssicherheit als Zustand definiert, in dem alle Menschen zu jeder Zeit ausreichend nahrhafte Lebensmittel zur Verfügung haben. Dennoch leiden noch immer mehr als eine Milliarde Menschen an Mangelernährung. Zudem ist die zukünftige Ernährungssicherheit bedroht, denn neben einer wachsenden Bevölkerung erzeugen auch veränderte Ernährungsgewohnheiten mit einem erhöhten Anteil tierischer Nahrungsmittel eine deutliche Zunahme des Nahrungsbedarfs. Gleichzeitig steht die landwirtschaftliche Produktion unter Herausforderungen, insbesondere durch den Klimawandel. Es ist von einer Zunahme der Klimaschwankungen und -extreme auszugehen, die zu deutlichen Ernteeinbußen führen können. Deshalb ist eine Quantifizierung des Klimaeinflußes auf die Landwirtschaft notwendig um eine rechtzeitige Anpassung zu ermöglichen. Ein wichtiges Werkzeug zur Bestimmung des klimatischen Einflusses auf Ernteerträge sind Ertragsmodelle, welche mathematische Beschreibungen von Pflanzenwachstum und -erträgen darstellen. Ertragsmodelle werden zwar laufend verbessert, doch gibt es noch erhebliche Lücken in der Modellierung. Die vorliegende Dissertation schlägt in vier Kapiteln Verbesserungen für Ertragsmodelle vor, um Ernteschwankungen und den Einfluss von Klimaextremen besser abzubilden.

Der erste Teil ist eine Metastudie zur Bewertung und Strukturierung von Literaturwissen über Pflanzenphysiologie. Die Studie verwendet eine selbst entwickelte Methode zum Aufbau eines enzyklopädischen Netzwerks, welches eine systematische Einordnung unstrukturierten Wissens über Einflüsse auf Erntepflanzen ermöglicht. Die Netzwerkstruktur wird verwendet, um Vorschläge zur Verbesserung von Ertragsmodellen abzuleiten. Zwei davon, Ozonschäden und extreme Temperaturen, werden in den folgenden Teilen behandelt.

Der zweite Teil enthält eine Abschätzung von Ozonschäden in historischen Ernteerträgen. Dafür wird ein neu entwickeltes Ozonmodul in das Ertragsmodell LPJmL eingebaut. Das erweiterte Modell wird verwendet um globale Ernteeinbußen bei Weizen und Soja durch Ozon abzuschätzen. Neben der Ozonkonzentration werden die Wasserverfügbarkeit, die Temperatur und die CO_2-Konzentration als Einflüsse auf die Ozonschädigung berücksichtigt.

Dies stellt eine Verbesserung gegenüber früheren Abschätzungen dar, die nur lineare Korrelationen zwischen Ozon und Ernten berücksichtigen. Die Analyse legt nahe, dass Ozon zu Ernteeinbußen von bis zu 50% führen kann und somit ein gravierendes Problem darstellt.

Der dritte Teil behandelt die Auswirkungen von hohen Temperaturen auf Ernteerträge in den USA. Im Zuge der globalen Erwärmung werden Hitzewellen wahrscheinlich häufiger auftreten. Deshalb müssen Ertragsmodelle für Aussagen über zukünftige Erträge deren Auswirkungen richtig abbilden - was aktuellen Modellen allerdings abgesprochen wird. Daher wird hier untersucht, inwieweit neun verbreitete Modelle die beobachteten Auswirkungen von hohen Temperaturen auf Mais, Soja und Weizen in den USA abbilden. Die Ergebnisse zeigen, dass das Modellkollektiv in der Lage ist, beobachtete Verluste quantitativ richtig zu berechnen. Die dabei verwendete Kombination von statistischen und prozessbasierten Modellen legt zudem Wasserstress als Ursache für die Ernteeinbußen nahe - und nicht direkte Hitzeschäden. Dadurch wird Bewässerung als mögliche Gegenmaßnahme gerechtfertigt, zumindest bis zu einer Temperaturschwelle von 36 °C, unterhalb welcher ausreichend Beobachtungen für eine verlässliche Aussage vorliegen. Weiterhin lassen die Ergebnisse vermuten, dass erhöhte CO_2-Konzentrationen die Ernteeinbußen nicht verringern können. Diese Vermutung steht im Gegensatz zu gegenwärtigen Überzeugungen und sollte in Experimenten weiter untersucht werden.

Der vierte Teil schließlich beschreibt ein statistisches Modell, mit dem sowohl der Anteil des Wetters an globalen Ernteschwankungen als auch der Einfluss individueller Wettergrößen während verschiedener Wachstumsphasen beziffert werden kann. Die Kenntnis dieser Größen ist entscheidend für die Entwicklung von Ernteversicherungen und die Projektion von zukünftigen Ernten. Dazu wird ein vorhandenes statistisches Modell, ausgehend von Ergebnissen der Metastudie, um zwei Variablen für Hitze und Frost erweitert. Mit dem erweiterten Modell wird der Anteil des Wetters an Ernteschwankungen bei Mais, Soja und Weizen auf global 15-42% beziffert. Der genaue Wert und dessen Verlässlichkeit hängen von der betrachteten Pflanze und der Qualität der verwendeten Erntedaten ab. Das Modell ist auch für die kurzfristige Vorhersage von Ernten während der Wachstumsperiode geeignet. Eine derartige Abschätzung kann ein Gegensteuern bei Problemen und eine bessere Erntelogistik ermöglichen. Die Ergebnisse zeigen über 50% Vorhersagekraft zwei Monate vor der Ernte in mehreren Ländern und erlauben eine Vertiefung des Ansatzes.

In der Gesamtschau stellt die vorliegende Arbeit die negativen Einflüsse von Ozon und hohen Temperaturen für die landwirtschaftliche Produktion und damit auch für die Ernährungssicherheit heraus. Verschiedene Ertragsmodelle werden verwendet und verbessert und dadurch die Vorteile der Anwendung mehrerer Modelltypen hervorgehoben. Perspektiven für eine weitergehende Forschung zu Ozon, extremer Hitze und der kurzfristigen Vorhersage von Erträgen werden abschließend vorgestellt.

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I dedicate this work to Katharina. Life is marvelous with you, and the best is yet to come.

Contents

1 Introduction

1.1 Agriculture is a cornerstone of food security

1.1.1 Agriculture is a story of success, but increasingly under pressure

Agriculture is a global success story. Yields have continuously been growing since the onset of agriculture, and particularly in the decades after the "Green Revolution" from the 1960's on (Evenson and Gollin, 2003; Godfray et al., 2010a; Hafner, 2003). Moreover, yields show relatively low inter-annual variability in many of the world's major producing countries (Osborne and Wheeler, 2013; Ray et al., 2015). In high-input farming systems, yield-to-seed ratios can reach up to 100, which means that one grain of seed becomes 100 grains of yield (Spiertz, 2012). As a result, food prices have fallen and the share of malnourished people has steadily declined (Godfray et al., 2010b). Eventually, the majority of the global population of seven billion is provisioned with sufficient food (Godfray et al., 2010b; Wheeler and Braun, 2013).

But this success story does not come without drawbacks. Positive yield trends of the past could not be maintained in recent decades in several countries (Grassini et al., 2013; Hafner, 2003). Crop production is prone to losses under unfavorable or extreme weather events, which reduces yield stability (Battisti and Naylor, 2009; Lobell et al., 2011b). Examples are the drop in French wheat and barley harvests in 2016 or the current devastating drought in East Africa since 2016. And extreme weathers are likely to occur more frequently with climate change (Rahmstorf and Coumou, 2011), posing a threat for future production. Additionally, there is a direct contribution of highly intensified agriculture and livestock keeping to climate change, which may create a negative feedback loop (Foley et al., 2011). Other negative impacts of agriculture on the environment, namely on water or soil quality and biodiversity, are increasingly perceived (Foley et al., 2011; Makowski et al., 2013). Furthermore, the global food system contains inefficiencies, as the following points illustrate. The number of malnourished people, lacking either food or sufficiently nutritious food, is still large with estimates ranging between 1 and 2 billion (Godfray et al., 2010b; Lobell et al., 2008; Spiertz, 2012; Wheeler and Braun, 2013). At the same time, a substantial share of global crops is lost to inefficiency or waste (Alexander et al., 2017). Additionally, the eating habits of people are shifting towards diets based on more animal products like milk or meat. This could distort a just allocation of agricultural production (Alexander et al., 2017; Foley et al., 2011). Increasing resistance of pests or weeds to treatments pose another challenge that is not easy to overcome (Godfray et al., 2010b). Land degradation, increasing pressure on land resources and in particular a growing world population are further constraints that may impede the establishment of an agricultural system that provides sufficient and nutritious food for everyone (Foley et al., 2011).

Reconciling these two stories of agriculture is of fundamental importance for a prospering planet in the long term (Foley et al., 2011). This implies strengthening the successful parts of agricultural management, making it more resilient against stress and decreasing negative implications for the environment. Research in agriculture is an indispensable part of this transformation process towards more sustainability. A major topic in research is to understand and quantify weather influences on crop production and variability. While weather is defined as the current status of the atmosphere, for example of temperature and precipitation, climate is defined as the long-term (usually 30 years) average of these weather conditions. Weather variability is known to exert substantial influence on yield variability (Battisti and Naylor, 2009; Lobell et al., 2011a; Ray et al., 2015; Schlenker and Roberts, 2009; Tack et al., 2015), and weather patterns will very likely become different under climate change. A thorough quantification of weather influences on yield variability is thus paramount for projecting agricultural production under different future climates. With this thesis I aim to contribute to such a quantification. In the following sections the role of agriculture for food security is further elaborated and threats for food security in the future are highlighted. Afterwards, crop models are introduced as tools to quantify the illustrated relations and it is detailed how this thesis contributes to improving such models.

1.1.2 Food security is strongly tied to agriculture

Global food security is defined as "all people, at all times, having physical, social and economic access to sufficient, safe and nutritious food which meets their dietary needs and food preferences for an active and healthy life" (Food and Agriculture Organization of the United Nations, 2017). To attain food security, preconditions on four dimensions need to be fulfilled: availability of production, stability of production and access conditions, access to food, and utilization of food (Schmidhuber and Tubiello, 2007). Availability depends on the production of a sufficient amount of calories and relies on livestock, oceans, ecosystems and agriculture (Godfray et al., 2010a). Livestock and oceans provide protein-rich food to humans, while ecosystems provide wild food. The primary contribution to availability, though, comes from agriculture since it provides 80% of the global amount of human calorie consumption (Portmann et al., 2010). Of these 80%, 62% are directly consumed by humans while 35% are used as livestock feed and 3% as bioenergy (Foley et al., 2011). Agricultural performance is thus decisive for attaining food security: if there is not enough production, there cannot be food security even if all other conditions were fulfilled. In contrast, even with sufficient availability, food security may not be achieved if there is mismanagement within the other three dimensions. The stability dimension implies the steadiness of availability and access to sufficient food and demands a low variability in production and labor- or health-related risks. Access to food implies the necessary economic and non-monetary resources to acquire the desired quantity of food. Utilization of food, finally, is only possible if its quality - with respect to nutrients and safety - and the health condition of a person allow to digest and physically utilize the acquired food. A sufficient availability of food within one nation is thus neither sufficient nor necessary for food security in this nation, as the examples of India (enough production, but food insecure regions) and Singapore (no production, but food secure) demonstrate (Schmidhuber and Tubiello, 2007).

This thesis treats the availability and stability dimensions of food security. The importance of these two dimensions is highlighted subsequently. A decreasing supply of food and increasing or highly volatile prices can lead to poverty, political instability and migration (Cai et al., 2016; Gilbert and Morgan, 2010; Godfray et al., 2010a; Godfray et al., 2010b; Headey and Fan, 2008; Ivanic and Martin, 2008; Schleussner et al., 2016a). This may impinge on all dimensions of food security, as the following events illustrate. The current drought in East Africa that began in 2016 has caused losses in agricultural production and livestock numbers, triggering severe livelihood crises (Food and Agriculture Organization of the United Nations, 2017). A second example is the food crisis in 2007/08 that led to upheavals in several low-income countries (Godfray et al., 2010a). In the 1970s, after severe harvest losses, the Soviet Union started to buy large amounts of US wheat reserves to avoid social unrest. This caused major price increases and global wheat shortages since this buying wave was unforeseen (Jones et al., 2016). Another well-studied example is the potato famine in Ireland in the mid 19th century. Massive harvest losses of potato due to a blight disease led to one million people dead and two million fleeing the country (O'Neill, 2010). Yet the total supply of food in Ireland was not scarce at that time: there were plenty of cereals harvested and livestock raised, but these rather went to export than to feed the home population (O'Neill, 2010). This proves that the access to food matters. All these examples demonstrate that a sufficient and stable agricultural production is of paramount importance for society, though the actual social or political impacts of production losses may be influenced by other factors like political management, commodity trade or the share of food diverted to uses like biodiesel or animal feed. It is thus vital to understand connections between the four dimensions of food security, to quantify the contribution of individual factors to them, and to anticipate problems. Only then can adequate counter-measures be taken and larger crises be precluded.

1.1.3 Future food security is under threat

The sufficiency of agricultural production is threatened by several factors: growing population, shift of dietary patterns, land degradation, increasing pressure on land resources and, above all, climate change. These threats to food security are schematically depicted in Figure 1.1. The global population is bound to increase to 9 billion people or more in this century (Bergaglio, 2016). Together with a dietary shift to more animal-based proteins in developing and transition countries, and the inherent conversion inefficiency from grains to meat, the demand for crop production is assumed to double within the 21st century (Spiertz, 2012). Even though the Green Revolution from the 1960s onwards has caused a large increase in global production (Evenson and Gollin, 2003), it is uncertain whether and under which efforts this positive trend can be sustained for the future (Fischer and Edmeades, 2010; Jaggard et al., 2010; Piesse and Thirtle, 2010). Criticism of unsustainable practices in intensive agriculture has also been growing (Evenson and Gollin, 2003; Foley et al., 2011), including the loss of productive areas due to land degradation (Amundson et al., 2015; Gibbs and Salmon, 2015; Gomiero, 2016). If demand is increasing and production increases becoming more difficult, the expansion of arable land could help to close the gap. Yet land expansion is constrained by the multiple functions of land: apart from food and fodder provision, land is also required for refuges for wild species, ecosystem services, recreational areas for humans and urban or road constructions. Furthermore, conversion of non-agricultural land to harvested fields is restricted by the environmental impacts of conversion, like the emission of greenhouse gases, which may outweigh short-term production gains in the long run (Foley et al., 2011). These constraints discredit land expansion as a quick solution for increasing production.

A major risk for future agricultural production is climate change. Anthropogenic climate change is the increase of global mean temperatures and shift of weather patterns caused by continued emission of greenhouse gases into the atmosphere (Stocker et al., 2013). With respect to food security, climate change will very likely impact on all four resources of food: agriculture, livestock, oceans and ecosystems (Field et al., 2014; Schmidhuber and Tubiello, 2007; Wheeler and Braun, 2013). Furthermore, all four dimensions of food security will be afflicted (Schmidhuber and Tubiello, 2007; Wheeler and Braun, 2013). The quantity of effects depends on the severity of climate change, the geographic region, the cropping system and the political framework (Rosenzweig et al., 2014; Rosenzweig and Tubiello, 2007). Yet some of the effects of climate change on crop production can already be observed today (Lobell et al., 2011b) or are very likely to occur in the near future (Lobell and Tebaldi, 2014). Examples of these are listed in the remainder of this paragraph. An increased concentration of carbon dioxide (CO_2) is a major cause of climate change. More CO_2 usually enables better plant growth since they require CO_2 as primary resource for carbon compounds (Deryng et al., 2016; Long et al., 2006). The co-effects of CO_2 as greenhouse gas, though, may more than offset these benefits. Additionally, a trade-off between increasing yields and maintaining nutritional values under rising CO_2 may render yield increases futile (Müller et al., 2014; Myers et al., 2014). Another effect of climate change is that, in mid and high latitudes, weather conditions suitable for crop growing will likely last longer both in spring and autumn (Reyes-Fox et al., 2014). This is usually beneficial for crops as they have more time to accumulate biomass and yield. Likewise, a poleward shift of regions apt for growing can be expected for temperate and tropical crops with a global increase of temperatures (Scheffers and De Meester, 2016). This may be beneficial for a few countries like Russia or Canada which can then grow crops that are, until now, limited by too cold temperatures. But these positive effects - longer and warmer seasons - for few countries may be more than offset by large negative effects in many other countries. Additionally, such positive effects can only be expected as long as climate change does not exceed a certain threshold (Field et al., 2014; Schleussner et al., 2016b). The negative effects of climate change include an increase in warmer days, which may entail large yield losses when formerly beneficial temperatures are replaced by detrimental ones (see chapter 4). Together with an expected increase in frequency and intensity of extreme temperature events this can severely diminish global production (Barnabás et al., 2008; Battisti and Naylor, 2009; Lobell et al., 2011a; Schlenker and Roberts, 2009; Tack et al., 2015). Precipitation patterns may as well be altered under climate change (Sillmann et al., 2013). This may increase the number and intensity of extreme events like drought spells or floods, which severely affect crop production (Barnabás et al., 2008; Thornton et al., 2014). Moreover, an increase of atmospheric pollutants may come along with climate change, though strongly dependent on emission scenario and the strength of pollution mitigation policies (Jacob and Winner, 2009; Rao et al., 2016). The detrimental influence of ozone on crop yields, as one major example, is illustrated in chapter 3. Finally, the prevalence of pest or disease outbreaks may shift with climate change, which can alter crop production substantially (Chakraborty and Newton, 2011; Hatfield et al., 2011).

Three pathways are usually followed to increase agricultural production: improvement or adaptation of crops, agricultural land expansion and intensified inputs. The first option, adaptation, implies the choice or creation of improved crops that can, for example, better cope with heat or drought stress. It is portrayed as a way to overcome some of the challenges mentioned above (Ewert, 2012; Lobell et al., 2008; Olmstead and Rhode, 2011; Varshney et al., 2011). But the speed and magnitude of change under unabated global warming may be more than adaptation may counteract (Olesen et al., 2011). Together with the restricted adaptation potential of current crops it seems reasonable not to trust in adaptation alone (Lobell et al., 2014; Lobell, 2014; Moore and Lobell, 2014; Schlenker and Roberts, 2009; Tack et al., 2015). Since agricultural land expansion, the second option for production increases, is restricted - as detailed above - a higher productivity on existing agricultural areas is mandatory. But the intensification of inputs, as third option, needs to be performed intelligently to avoid further environmental damage (Foley et al., 2011; Godfray et al., 2010b; Lipper et al., 2014; West et al., 2010). Apart from production increases, commodity trade is often considered an option to balance regional supply and demand differences. But it is uncertain whether trade can buffer the shifts in crop productivities (Baldos and Hertel, 2015; Godfray et al., 2010b; Paini et al., 2016; Spiertz, 2012; Suweis et al., 2015).

In brief, many challenges need to be addressed for maintaining or improving agricultural production and thus food security in the 21st century. A prerequisite for sustained agricultural production is an improved understanding and quantification of environmental influences on crop yields. This may support plant breeding for changing conditions, the establishment of early warning systems to anticipate problems and the adaptation of production systems in terms of cultivar choice or growing season management. Major tools to support these processes by acquiring and validating knowledge in crop-environment relations, and by quantifying their importance for agricultural production, are crop models. The next section provides an introduction to these models and their potential uses.

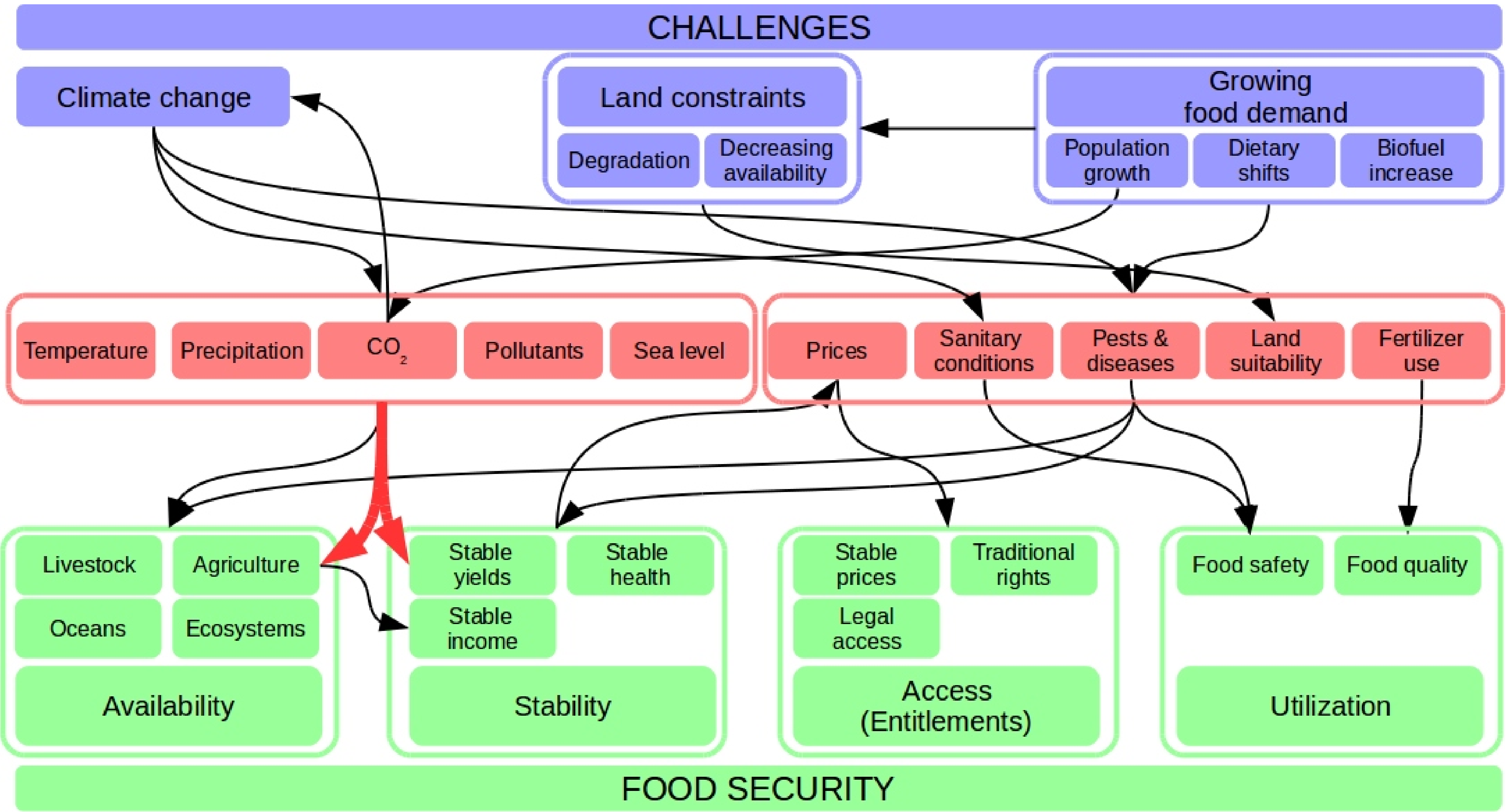

Figure 1.1: Interactions between the four dimensions of food security (green boxes) and three major challenges (magenta boxes). Influences are mediated by physical or economic effectors (light red boxes). The depicted interactions are an author's (sparse) selection of major influences out of the manifold complex dependencies and are based on Godfray et al. (2010a), Godfray et al. (2010b), Schmidhuber and Tubiello (2007), and Spiertz (2012). Note that CO_2 is actually a driver of climate change, but is set here among other climate variables due to its influence on crop growth, ecosystems and ocean chemistry. The two thick red arrows mark the scope of this thesis: to characterize influences of climate on availability and stability of agricultural production.

1.2 Crop models are major tools to estimate agricultural production

1.2.1 Crop models simulate influences of environmental conditions on crop growth

Experiments in chambers or on fields are of eminent importance for understanding plant physiology. However, they are usually performed for only one or few variations of cultivar, location or growing conditions. This makes it difficult to derive effects for larger scales. Crop models, instead, can interpolate between different experimental results by abstraction to equations (Boote et al., 2013; Ewert et al., 2015; Hansen and Jones, 2000; Jones et al., 2016). They support the quantification of crop responses to diverse environmental conditions, which is particularly relevant under climate change when weather patterns shift and extreme events are likely to increase (Rahmstorf and Coumou, 2011; Sillmann et al., 2013; Stocker et al., 2013). Crop models in this context are defined as mathematical formulations that quantitatively simulate carbon, nitrogen and/or water cycles to calculate crop attributes like yield, biomass or leaf chlorophyll amount, from quantitative inputs including weather data or soil properties.

Crop modeling looks back on a history of more than 50 years. The development from early prototypes to highly advanced global cropping system simulations is reviewed in Boote et al. (2013), Ewert et al. (2015), Holzworth et al. (2015), and Jones et al. (2016). Crop models have either been designed for advancing the knowledge on crops and their environment or for providing guidance in farming practice or policy (Jones et al., 2016; Paola et al., 2016). They can support decision planning on farm level, plant breeding, efficient resource usage, yield gap analyses or the evaluation of policy measures (Holzworth et al., 2015). Crop models are also used to study large-scale effects of different climates, management practices, land-use allocations or adaptation measures on agricultural production (White et al., 2011). Furthermore, their results can be used to assess three dimensions of food security. First, the availability of food can be estimated directly by the amount of simulated production. Second, the stability of yields, in dependence of weather or other factors, can be derived from the variability of simulated yields. Third, the economic access to food can be gauged by using simulated yields as input to economic models, which can then be applied to calculate food prices. An exemplary chain of models and outputs is depicted in Figure 1.2.

Models exist on different geographical scales, from individual plants to the globe, and regarding their construction principles they can be coarsely classified into two different types: statistical and process-based (Lobell and Asseng, 2017; Lobell and Burke, 2010; Paola et al., 2016). Hybrids between these two types exist, too, aiming to reconcile advantages

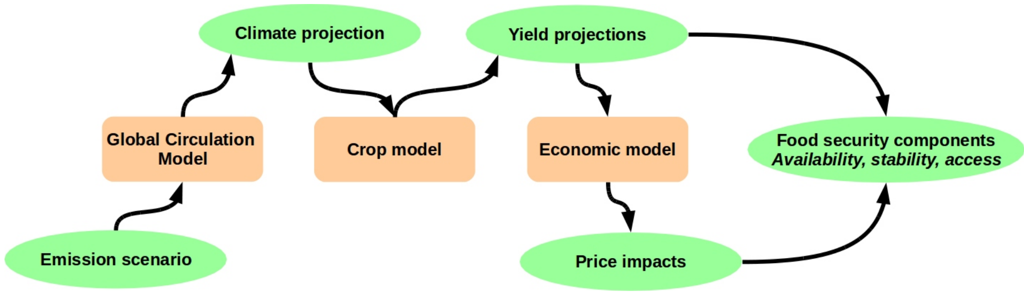

Figure 1.2: Modeling chain to assess three dimensions of future food security under an exogenous emission scenario. Global Circulation Models can project future climate from emissions. This climate is fed into crop models to estimate future yields. Their amount and variability can be utilized to assess parts of the availability and stability dimensions. A further calculation of food prices with economic models, given yield projections and exogenous socio-economic factors, may support projections on the economic access dimension of future food security.

from both methods (Paola et al., 2016). Statistical models are usually based on regression methods relating yield or another variable of interest to growing conditions. Their complexity can range from simple correlations of yield with aggregate temperature and precipitation (e.g. Ray et al. (2015)) to models with several tens of variables and interactions (Blanc, 2017; McGrath et al., 2015). Process-based models, in contrast, take a different approach by explicitly simulating physiological reactions like carbon assimilation, root growth or leaf formation. The results of these reactions are integrated from small time steps, usually hours or days, to the full growing season.

Both model types come with idiosyncratic advantages and disadvantages; the list here is based on Gornott and Wechsung (2016), Jones et al. (2016), Lobell and Asseng (2017), and Lobell and Burke (2010). Statistical models are mostly simple to construct and calculate, though sometimes with statistical intricacies. They do not require any further input data except for the exogenous and endogenous variables contained in the model. Moreover, statistical models of weather influence on yields are deemed to capture also indirect effects of weather, like pests and diseases, as the abstraction level is coarse enough to subsume these influences in their coefficients. However, linear statistical models are usually not able to capture non-linear effects like strong yield losses from a heat or cold wave. It is, in general, difficult to estimate effects outside the training scope. Co-linearity of exogenous variables may confound results if not enough training data are available to resolve dependencies. Additionally, mechanistic explanations of exogenous influences are lacking and intermediate variables, for example leaf biomass or root penetration depth, are not available. Sub-seasonal influences of variables are not captured if only growing-season aggregates of the values are fed into the model. Finally, projections of future yields under a changing climate are difficult since CO_2, one of the major uncertainties in this task, is usually not considered (Estes et al., 2013). There exist statistical techniques to make up for each of these deficiencies,

but these can involve intricacies in modeling and result interpretation, thus nullifying the major advantage of simplicity.
Process-based models, in contrast, aim to overcome these drawbacks. Virtues depend on the specific model, but usually this type enables capturing non-linear effects, in particular also during the growing season, by using a finer time step of days or hours. Intermediate variables are available for inspection which allows for more detailed hypotheses about physiological mechanisms. Future projections including changing CO_2 concentrations are possible because the required photosynthesis dynamics are usually implemented (on different scales of complexity, though). Effects of simultaneous changes of several variables, also outside the training scope, can be simulated with process-based models since they include broad mechanistic descriptions that are usually based on manifold experimental observations. The disadvantages of process-based models, however, include their high programming effort and the requirement of many physiological parameters for the process descriptions, which can involve complex calibration routines. The lacking ability to capture indirect effects which are not explicitly modeled is stated as a further deficit of this model type. Moreover, a missing or only weak consideration of extreme climate effects is seen as a drawback, since process-based models were not originally designed for climate change assessments (Lobell and Asseng, 2017; Rötter et al., 2011).

To overcome model-specific drawbacks, the usage of model ensembles, with one or both model types, has recently gained momentum and is an elegant method to frame uncertainties (Asseng et al., 2015; Estes et al., 2013; Liu et al., 2016; Lobell and Asseng, 2017; Rötter et al., 2011). It allows profiting from different model types and divergent modes of implementation, since no single model can fulfill all the ascribed virtues listed above. In this thesis I follow the ensemble approach and use models of different types: a process-based model is amended in chapter 3, a statistical model is amended in chapter 5, and in chapter 4 a combination of statistical and process-based models is utilized to gain new mechanistic insights.

1.2.2 Crop models require improvements

When crop models are used to project future yields under climate change, it is important to know how much one can trust their projections. Therefore the uncertainty of projections needs to be quantified. This is usually achieved by comparing historical simulations with observed yields.

Recent such comparisons between models and observations have revealed that there is substantial divergence between models in terms of explained yield variance, impacts, process importance and input weighting (Asseng et al., 2015; Folberth et al., 2016; Frieler et al., 2017; Müller et al., 2017). The divergent performance across models is illustrated in Figure 1.3, showing the correlation between observed and simulated global yield time series for wheat. It

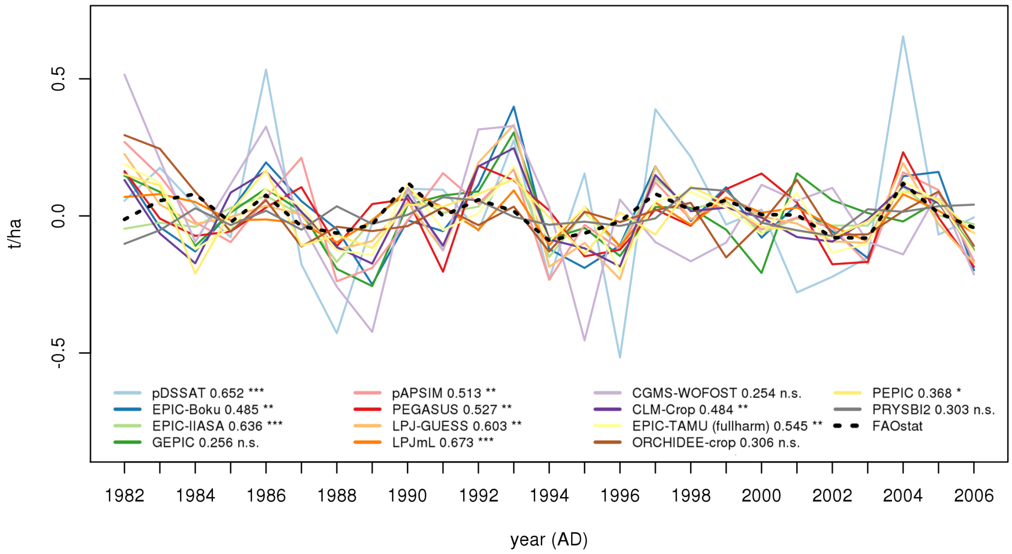

Figure 1.3: De-trended time series of global wheat yield variability from 1982 to 2006 as observed or modeled by different crop models. Observed yield variability reported by FAO is indicated by the dashed black line, while simulated time series are shown in colors. The correlation coefficients between simulation and observation (Pearson's r) and their significance (*** for $p < 0.001$, ** for $p < 0.05$, * for $p < 0.1$, n.s. for not significant) for individual models are provided below the time lines. Figure is taken with courtesy from Müller et al. (2017).

is taken from Müller et al. (2017), where a profound intercomparison of 14 different process-based crop models was performed, and demonstrates current skills and deficiencies of crop models. All models in the intercomparison are driven by the same daily weather input, while other settings like soil attributes, fertilization or management decisions are constant over time (detailed simulation settings are described in Elliott et al. (2015) and Müller et al. (2017)). Thus, the correlation between observed and simulated yields provides an estimate of the purely *weather-driven* share of observed yield variability. For this reason, a perfect agreement cannot be expected; the fraction of weather-driven global yield variability is estimated elsewhere around one third (Ray et al., 2015). But the divergence between crop models is striking: seven models achieve a Pearson's r value above 0.5, indicating substantial influence of weather on yields, while four models do not find any significant correlation. Low and high yield values do not match between observations and simulations for all cases and the variability of yields is grossly overestimated by several models. The question therefore is about the cause of these differences: which share of unexplained variance is due to a lacking influence of weather (and thus should not be captured by weather-driven models), and which share is due to model deficiencies? Assuming that the true influence of weather is unknown, one can only start asking which effects are captured well in some models, but not in others, and which effects are completely missing in all models. In Müller et al. (2017) the authors do not distill explicit improvements suggestions, but identify high quality input data of, for example, soil, fertilizer management or growing seasons as critical for model evaluations and ameliorations. Meanwhile, candidate processes for model improvements have been identified in several expert-based summaries, for example Boote et al. (2013), Ewert et al. (2015), Holzworth et al. (2015), and Rötter et al. (2011). Prominent candidates are the response of yields to extreme weather like heat, drought or flood, the cycling of nutrients, crop losses by pests and diseases and the quantity of the CO_2 fertilization effect. The inclusion of nutritional values and the broadening of the spectrum of crops is also demanded. Additionally, the linkage between crop models and economic models, though having improved in recent years, still requires investment in crop models to allow for seamless integration. These amendments may be required to enhance skills of current models and to allow for even broader applications. In this thesis, I pursue some of these suggestions, which are detailed in the next section.

1.3 This thesis treats four research questions

With this dissertation I aim to contribute to improving crop models with respect to better modeling of yield variability. My research questions are deduced from the current structure of knowledge about plant physiology, which is available in three different forms: experimental results, scientific articles and crop models. These domains are overlapping, but there is abundant knowledge in the literature, including published experimental results, that is not yet present in crop models and could help to improve them. Therefore I start with a structuring of the literature knowledge to derive strategies for model improvement, independent from previous reviews (chapter two). In the subsequent chapters, one improvement strategy is selected as suggested by the newly constructed knowledge structure. The selected strategy, which corresponds to a physiological process, is then either included into an existing crop model (ozone in chapter three and extreme temperatures in chapter five) or an ensemble of crop models is tested how well they already contain this process (high temperatures in chapter four). In more detail, my research questions are as follows.

1. The second chapter explores how published knowledge about physiological influences on crop yields can systematically be harmonized, and how this harmonized knowledge base can be used to derive suggestions for crop model improvements. To this end, a meta-study of literature knowledge is presented that pursues both tasks. Its methods include a manual literature mining and a semi-quantitative network analysis that enables the systematic treatment of environmental influences on crop yields. Suggestions for crop model amendments are derived based on the network structure. The method is new and adopts a perspective between experiments (as described in the literature)

and models. Two pathways for model improvement that emerge from the meta-study, namely ozone and extreme temperatures, are treated in the subsequent chapters.

2. Following one suggestion derived from the meta-study, the third chapter analyzes the extent to which historical crop yields have suffered from ozone pollution. To answer this question, an ozone-damage module is implemented in the global vegetation model LPJmL (chapter three). The enhanced model is used to simulate historical global wheat and soybean yield losses from ozone pollution. The ozone module introduced here is a novel development integrating experimental findings, scaling them up to the global level and considering co-variates of ozone damage like water, temperature and CO_2. The latter is an advancement over previous assessments that only considered linear relations between ozone and yield.
3. High temperatures are known as a major cause for yield losses, as portrayed in the meta-study. But it has recently been doubted whether crop models are able to correctly simulate the effects of heat stress on crops. Therefore chapter four assesses, first, to what extent state-of-the-art crop models can reproduce observed effects of high temperatures in the US and, second, what this implies for future US yields. The utilized combination of statistical and process-based models is new and allows for mechanistic insights that were not possible before. The USA are used as an application case due to the extensive data base on crop yields and their large contribution to global crop production.
4. Chapter five extends an existing statistical model by extreme temperature penalties - as suggested by the meta-study - and applies it globally for staple crops. The quantification of weather influence on global crop yields is necessary to estimate future yields under climate change. The choice of a statistical model enables such a global quantification of yield variability with limited input data that is both fast and robust. The method also allows for forecasting of crop yields within the growing season, which is considered a major instrument to anticipate and buffer yield losses and thus enhance local food security.

The final chapter synthesizes the findings from the four individual studies, places them in a broader context and concludes with perspectives for further research. My contributions to the studies in chapters 2 to 5 are as follows.

1. The literature mining study in chapter two is based on a suggestion by Christoph Müller[1] to re-valorize existing literature, with the aim to derive suggestions for crop model improvements. I developed the method and the design of the study. I performed the required literature mining, implemented the method and wrote the manuscript. Susanne Rolinski and Christoph Müller supported me in the whole process.
2. The study about ozone damages on crops in chapter three is based on results from the meta-study. Ozone was identified by myself as one possible avenue for improving crop

[1]Co-author affiliations are reported in the respective studies.

models towards more realistic yield assessments. Thus I designed and implemented an ozone damage module for LPJmL. I performed the required literature search, designed the layout of the study and wrote the manuscript. Susanne Rolinski, Sibyll Schaphoff and Christoph Müller supported me in the whole process.

3. The study about the representation of high-temperature effects in crop models in chapter four is based on an idea by Katja Frieler. The aim was to evaluate whether crop models, participating in the ISI-MIP and AgMIP projects, can reproduce observed effects of high temperatures on crops. The temperature-exposure regression used as evaluation tool was developed by Wolfram Schlenker. I designed and performed the study and wrote the manuscript together with Katja Frieler. Additional support was provided by Christoph Müller and Joshua Elliott. All other co-authors provided model results under the auspices of the AgMIP and ISI-MIP projects and/or commented on the manuscript.
4. The study about the global application of a semi-empirical model was initiated by Frank Wechsung. I designed the study together with Frank Wechsung, with additional contributions by Christoph Gornott. I performed the study and wrote the manuscript with support from both co-authors.

Chapters 2, 4 and 5 of this thesis are reproductions of peer-reviewed and published scientific articles. The study about global ozone damages (chapter three) has been submitted to Global Change Biology on June 08, 2017 and has been sent our for review. As a co-author, I contributed to further manuscripts; an overview of all articles is provided in Table 1.1.

Table 1.1: Selection of scientific publications that I contributed to during my thesis.

Nr	Title	Thesis chapter	Author position	Status	Journal (Year)	DOI
1	A network-based approach for semi-quantitative knowledge mining and its application to yield variability	2	1	published	Environmental Research Letters (2016)	10.1088/1748-9326/11/12/123001
2	Global historical soybean and wheat yield loss estimates from ozone pollution considering water and temperature as modifying effects	3	1	under review	Global Change Biology	n.a.
3	Consistent negative response of US crops to high temperatures in observations and crop models	4	1	published	Nature Communications (2017)	10.1038/ncomms13931
4	Global evaluation of a semi-empirical model for yield anomalies and application to within-season yield forecasting	5	1	published	Global Change Biology (2017)	10.1111/gcb.13738
5	Understanding the weather-signal in national crop-yield variability	n.a.	2	published	Earth's Future (2017)	10.1002/2016EF000525
6	The critical role of the routing scheme in simulating peak river discharge in global hydrological models	n.a.	7	published	Environmental Research Letters (2017)	10.1088/1748-9326/aa7250
7	French crop yield, area and production from 1900 to 2013 on department resolution	n.a.	1	in preparation	Nature Scientific Data	
8	Process representation is key to future crop yield projections	n.a.	2	in preparation	Earth System Dynamics	
9	On deeper human dimensions in earth system analysis	n.a.	2	in preparation	Earth System Dynamics	

2 A network-based approach for semi-quantitative knowledge mining

This chapter is a reproduction of the article published as "Schauberger, Rolinski & Müller: A network-based approach for semi-quantitative knowledge mining and its application to yield variability, Environmental Research Letters 11, 2016". The article DOI is 10.1088/1748-9326/11/12/123001.

2.1 Article

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TOPICAL REVIEW

A network-based approach for semi-quantitative knowledge mining and its application to yield variability

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Keywords: yield variability, crop models, interaction network, plant process, wheat, maize, rice

Supplementary material for this article is available online

Abstract

Variability of crop yields is detrimental for food security. Under climate change its amplitude is likely to increase, thus it is essential to understand the underlying causes and mechanisms. Crop models are the primary tool to project future changes in crop yields under climate change. A systematic overview of drivers and mechanisms of crop yield variability (YV) can thus inform crop model development and facilitate improved understanding of climate change impacts on crop yields. Yet there is a vast body of literature on crop physiology and YV, which makes a prioritization of mechanisms for implementation in models challenging. Therefore this paper takes on a novel approach to systematically mine and organize existing knowledge from the literature. The aim is to identify important mechanisms lacking in models, which can help to set priorities in model improvement. We structure knowledge from the literature in a semi-quantitative network. This network consists of complex interactions between growing conditions, plant physiology and crop yield. We utilize the resulting network structure to assign relative importance to causes of YV and related plant physiological processes. As expected, our findings confirm existing knowledge, in particular on the dominant role of temperature and precipitation, but also highlight other important drivers of YV. More importantly, our method allows for identifying the relevant physiological processes that transmit variability in growing conditions to variability in yield. We can identify explicit targets for the improvement of crop models. The network can additionally guide model development by outlining complex interactions between processes and by easily retrieving quantitative information for each of the 350 interactions. We show the validity of our network method as a structured, consistent and scalable dictionary of literature. The method can easily be applied to many other research fields.

1. Introduction

Crop yields can vary strongly between years and locations. These fluctuations, or yield variability (YV), are undesirable, since they undermine food security on three dimensions (Morton 2007, Schmidhuber and Tubiello 2007, Wheeler and von Braun 2013, Thornton *et al* 2014). First, the amount of harvested food can be lower than necessary, second, the financial sustainability of farming systems can be challenged, and third, the access to nutritious food can be diminished by rising prices or export bans connected to variable yields (Headey and Fan 2008, Headey 2010, Coumou and Rahmstorf 2012, Chung *et al* 2014). Substantial fractions of historic YV can be explained by weather variability and extremes like droughts, floods, heat waves, cold spells, or combinations of them (Porter and Semenov 2005, Schlenker and Roberts 2009, Coumou and Rahmstorf 2012, Lobell *et al* 2013, Deryng *et al* 2014, Ray *et al* 2015, Lesk *et al* 2016). Globally about one third of YV can be explained by weather variation, but with large regional differences (Ray *et al* 2015). Although some of the actual weather-induced variation in yields might be lost in the aggregation procedure, this leaves up to two thirds of YV to be explained (SI figure S1). Thus other environmental or management factors must cause the variation. An example for regional differences is the

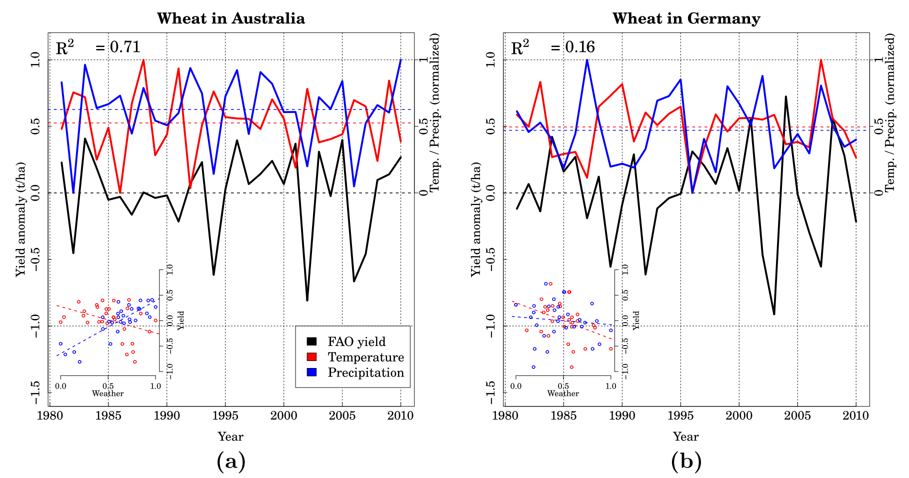

Figure 1. Observed yield anomaly time series from 1981 to 2010 (black lines) for wheat in Australia (a) and Germany (b) (FAO 2015). Temperature and precipitation (taken from the AgMERRA climate data set (Ruane *et al* 2015) at 0.5° spatial resolution, weighted and aggregated nationally by MIRCA2000 land-use patterns (Portmann *et al* 2010) and normalized to [0-1]) are displayed as red and blue lines, respectively; the dashed lines are their mean values. The R^2 values indicate the explained variance by the regression model 'Yield $= \alpha + \beta * $ Temperature $+ \gamma *$ Precipitation $+ \epsilon$'. The inlays display the correlation between yield anomaly and normalized weather variables; dashed lines are slopes of linear correlations.

influence of precipitation on YV (figure 1). Precipitation variability clearly determines wheat variability in Australia (panel (a) with inlay), while in Germany wheat does not exhibit a clear, simple response to either temperature or precipitation (panel (b); Ray *et al* 2015).

Variability in growing conditions is transmitted to yield levels by plant physiological processes. These form a layer of complexity that has to be accounted for when assessing future YV. A huge body of experimentally-derived knowledge describes quantitative relationships between growing conditions, plant physiological processes and yield (e.g. Barnabás *et al* 2008, Farooq *et al* 2009b, Hatfield *et al* 2011). Process-based crop models are frequently used to study the influence of growing conditions on crop physiology and yields apart from experiments. These models represent our current knowledge on plant interactions with their environment (Boote *et al* 2013, Holzworth *et al* 2015). They are apt to reliably reproduce spatially aggregated mean yield levels (Palosuo *et al* 2011, Asseng *et al* 2015, Martre *et al* 2015).

Despite the abundant knowledge about YV a consistent and comprehensive overview of its causes and mechanisms is not yet available. Apart from the study by Ray *et al* (2015) and similar predecessors (see references therein) other causes of YV were also researched, but focusing on subsets of possible causes only. Bakker *et al* (2005) decipher the contribution of soil, climate and management as important sources of spatial wheat YV in Europe. Porter and Semenov (2005) or Asseng *et al* (2011) consider the impacts of heat stress on crop yields, but do not consider other climatic factors like water or solar radiation, or do not discuss plant physiological processes. Other studies include Yu *et al* (2014), who identify temporal patterns of climate effects on wheat YV in Australia but do not consider processes, or Thornton *et al* (2014), who stress the importance of considering climate variability in food security assessments, and Ben-Ari and Makowski (2014), who identify the geographical distribution of crops as source of YV. At the same time crop models are deemed to lack adequate implementations of temporal YV under changing growing conditions (Rötter *et al* 2011, Sánchez *et al* 2014). In particular, extreme events like heat or drought have been found to be less well represented (Palosuo *et al* 2011, Rötter *et al* 2011, White *et al* 2011, Boote *et al* 2013, Rötter 2014, Asseng *et al* 2015). A comprehensive overview of the current status of crop models is provided by Boote *et al* (2013), who list nine cardinal points on how to improve crop models. Yet YV is not explicitly addressed as a topic, and stresses are only considered for heat, nitrogen and water. In Holzworth *et al* (2015) the authors state the effects of increased CO_2, temperature extremes, pests and hydrology as inadequately represented in models. Barlow *et al* (2015) and Eyshi Rezaei *et al* (2014) describe the negative effects of frost or heat on cereals and derive modeling guidelines. We conclude that a comprehensive and systematic overview of causes and mechanisms of YV is much needed, in particular for selecting suitable process candidates for model improvement.

Therefore we systematically review the literature on YV, and provide specific recommendations on how to incorporate the findings into process-based crop models. We adopt a novel, semi-quantitative technique for systematic reviews since the literature on plant physiology is overwhelming (more than 11 000 hits in the Web of Science[2] database for 'crop variability'). The idea is to structure knowledge in a network of interactions, where management, weather and other environmental factors define crop yield via plant physiological processes (figure 3). We then rank the possible contribution of individual growing parameters to yield from their location in the network topology, independent from their frequency in the literature. Furthermore, we quantify the importance of plant physiological processes for the transmission of variability in growing conditions to YV. Finally, we use this knowledge to compile suggestions for the improved representation of YV in crop models. The method is 'semi-quantitative' since we do not employ quantitative relationships between growing conditions and yield. But we do quantify the impact of growing condition parameters and plant physiological processes by their contribution to the network structure. To test the validity of the method we compare our proposals to the agenda suggested by Boote *et al* (2013). We consider maize (a C_4 plant), rice and wheat (both C_3 plants), representing roughly 92% of the globally harvested cereals (Ben-Ari and Makowski 2014) and planted on 41.3% of the global agricultural area (Portmann *et al* 2010).

This article describes a new method for mining knowledge from the literature, which is applied to review physiological mechanisms of YV. It is bound to reproduce existing knowledge to a large extent, but will check this for comprehensiveness and can thus guide future crop model development. With this review, we aim to answer three questions. First, what are key drivers of YV in wheat, maize and rice? Second, what are the central plant physiological processes involved? Third, how can the important interactions be included into crop models?

2. Materials and methods

2.1. Definitions and network terminology

Yield is an aggregate measure of crop characteristics and performance over the entire growing season. Yield can be defined as the integral of many short-term variations in growing conditions during the growing season and the plant's reaction towards them. Temporal YV is hence the variability of this integral (equation (2.1)). We define YV as average changes in absolute yield amounts (e.g. t/ha) between growing seasons of the same crop at the same location; an example measure would be the standard deviation.

$$\Delta\text{Yield} := \Delta\left[\int_{\text{growing season}} \text{physiological processes (growing conditions)}\right]. \tag{2.1}$$

[2] http://apps.webofknowledge.com/; accessed on 11 October 2015.

We focus on the fine-grain interactions between growing conditions, plant physiological processes and yield. Spatial variability plays, next to variability over time, a decisive role (Ben-Ari and Makowski 2014). Here we assume that spatial and temporal variation share common causes like e.g. temperature variation over space or time (Blois *et al* 2013), such that our analysis is also valid for spatial YV. We do not consider long-term trends, including a gradual increase in yields through improved management or a shift in yield trends from changes in climatic conditions. We use the term 'stress' to describe any non-optimal growing condition (e.g. a heat wave). Finally, plant growth and plant development ('phenology') are two distinct terms: while the first is a physical accumulation of biomass over the growing season, the latter refers to advances in developmental stages, for example the transition from vegetative to reproductive growth.

A network consists of *nodes* (i.e. elements) and *edges* between these. In our case nodes refer to processes, drivers or variables and edges to interactions between them. The *source/target node* of an edge is its starting/end point, respectively. A *path q* from node A to node B, denoted as $A \xrightarrow{q} B$, through the network follows a direction and can be direct (i.e. connecting A with B immediately) or indirect (i.e. containing intermediate nodes). The *path length* $|q|$ is the number of edges it contains (illustration in SI figure S2).

2.2. Network construction

The starting point for the network construction was the basic network scheme shown in figure 3, into which subcategories and interactions were subsequently added. The interactions described in six standard physiology text books (Hay and Walker 1989, Porter and Lawlor 1991, Hall *et al* 1993, Larcher 1995, Hay and Porter 2006, Lambers *et al* 2008) were used to add details: the network was refined with every encountered subcategory or interaction. For example, if the scanned literature stated an influence of temperature (T) on photosynthesis, these two nodes were created (if not yet existent) and an interaction arrow drawn from T to photosynthesis (if not yet existent). If an interaction edge was already present, the new reference was recorded, but no duplicate edge was included. This ensures that interactions do not gain more weight just because they are frequently stated in the literature. With more details, the categories were subdivided. For each node and interaction it was annotated for which crop (wheat/maize/rice or all three) it is valid, thus creating crop-specific networks.

Afterwards a systematic search for studies in the full ISI Web of Science database[3] was performed. A keyword list with 55 entries was created, using terms from the initial textbook-based network. General terms like '*yield variability*' and more specific ones like '*temperature AND wheat AND yield*' were included (full keyword list in SI table S3). Only papers after 1990 were considered to limit the number of search results. This first search for the keywords in the 'Topic' fields yielded 460 765 studies in total, so the results were filtered to contain only 'Review' papers. If this number was still large (> 200) for one search term the results were further filtered to contain the keywords in the 'Title' instead of 'Topic' (with few exceptions; SI table S3). Additionally, references to and in four large reviews (Barnabás *et al* 2008, Farooq *et al* 2009b, Hatfield *et al* 2011, Boote *et al* 2013) were searched to validate the efficacy of the keyword approach. These search criteria resulted in 8818 studies that were inspected for relevance by sequentially looking at title, abstract and full text. An article was *relevant* if the study included an explicit treatment of plant physiological processes, with either growing condition influences on them or their influence on yield, and the interactions were not derived solely from modeling studies. More recent studies were selected when similar but older ones existed. Molecular details like enzyme activity or signaling molecules and genotypic or cultivar-specific differences are not considered. After this final filter step, 60 relevant papers remained from which interactions were manually included in the initial text book-based network.

Six out of 350 edges were added without explicit literature reference as they were considered obvious but have not been found in the selected literature. These are: irrigation adds to soil water content (SWC), fertilization adds to soil nutrient levels, sowing and harvesting time affect the amount of precipitation and solar radiation intercepted during the growing season, water uptake is affected by SWC, and the plant's uptake of micronutrients influences their content in grains.

2.3. Driver and process importance

The importance of drivers as possible sources of YV was derived from the network structure. The importance of a driver d is defined by the number of different paths from d to yield amount, mediated by various plant physiological processes (equation (2.2); m denotes the maximum path length).

$$\text{importance}_m(d) := |\{q \mid d \xrightarrow{q} \text{Yield} \wedge |q| \leqslant m\}|. \tag{2.2}$$

A maximum path length $m = 4$ (i.e. at most three intermediate nodes) was chosen. This allows for possibly important indirect effects but avoids cyclic paths. Sensitivity to this assumption was tested with path lengths from 1 to 10. Each interaction was counted only once, independent of the number of studies which mentioned that specific influence. Thus a frequent occurrence of an interaction in the literature does not necessarily imply a high ranking. It is assumed that only drivers that exert substantial impact on plant physiology *and* are variable in nature can cause YV. Therefore each possible driver was qualitatively classified for its variability in nature and drivers with low variation were excluded. Three reduced network variants were also analyzed to search for variability drivers other than temperature (T) and precipitation (Pr). From the full network either T (air and soil, with all out-edges), or Pr along with SWC, or both T and Pr nodes (then also air humidity) were deleted; then the importance assessment was repeated.

The importance of a process for transmitting variability in growing conditions to YV was evaluated by plotting both impact values against each other (scheme in figure 2). The *impact* of a node v on another node w is defined by the number of paths between v and w, similar to the importance of drivers in equation (2.2). A process which is impacted by many different influences from the growing conditions (above the mean value on x-axis) and in turn substantially impacts yield levels (above mean value of y-axis) was assumed *important* in this respect. Processes in the other sectors of the plot did fulfill either one criterion or none at all, and were thus deemed less or not important for shaping yield amounts.

We consider this network method as 'semi-quantitative' since quantitative relationships between growing conditions and yield are not included, but the relative impact of growing condition parameters and plant physiological processes is evaluated by their quantitative contribution to the network structure.

The network approach explicitly integrates across physiological scales and assumes that driver or process importance is directly related to their number of network links to yield. The adequacy of these two assumptions is justified in the discussion section.

3. Results

3.1. Network structure

The crop yield interaction network contains 130 nodes and 509 edges. Of the edges 350 are interactions between nodes (*functional interactions*); the other edges only connect hierarchical distinctions in categories, e.g. 'uptake' to 'uptake of nutrients'. Each node is connected on average by 3.92 edges (functional edges only: 2.69), the average number of studies cited

[3] http://apps.webofknowledge.com/; accession dates in SI table S3.

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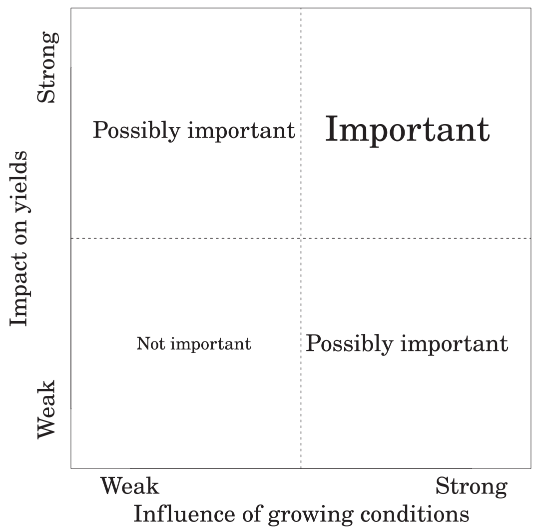

Figure 2. Evaluation scheme for the importance of plant physiological processes. Processes that are strongly influenced by growing conditions and in turn also exert an intense effect on yields can be considered as putatively important for transmitting variability from the growing conditions to yield levels. These will gather in the upper right corner. Dashed threshold lines are value means for each axis.

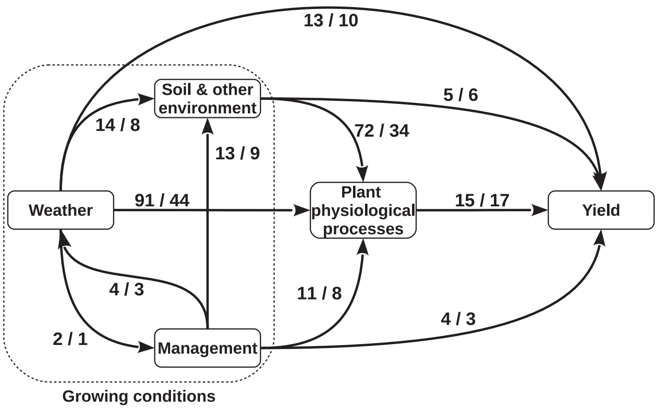

Figure 3. Condensed interaction network. Each edge between the five major categories (rounded boxes) is annotated with the number of interactions between the corresponding subcategories (self-edges are not counted), and the number of distinct studies cited. The full network can be found in SI figure S3.

per functional interaction is 1.53, and the nodes with the highest out-degree are temperature (49 out-edges), SWC (39) and CO_2 (26). The number of edge annotations for only wheat are 105, for only maize 36 and for only rice 32; interaction references applying to all three crops summarize to 363 (SI table S1). A condensed version of the network is shown in figure 3 where interaction and citation numbers are split between categories. The full interaction network is provided in the SI (figure S3 and as GraphML editable network file). Among the drivers of YV in growing conditions we considered the following stressors: chilliness and heat, water logging and drought, excess and shortage of solar radiation, ozone, strong wind, nutrient shortage and excess, salt and acidity stress, pests and diseases, and toxic substances.

3.2. Relative importance of factors causing YV

SWC, with its climatic precursor precipitation (Pr), and temperature (T) are ranked as foremost influences on yield by our method. An analysis of the full and the reduced network variants suggests also the following environmental factors as physiologically important for

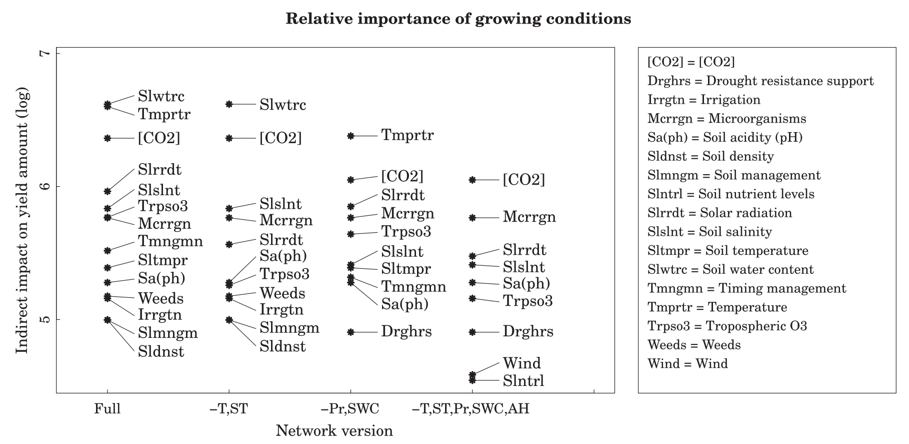

Figure 4. Relative importance of growing condition parameters for yield amount in all three crops, measured as the number of indirect interactions between driver and yield amount up to a path length of four (on *y*-axis, log scale). Four network subtypes (on *x*-axis) were analyzed: full ('Full'), without temperature in air and soil ('- T,ST'), without precipitation and soil water content ('- Pr,SWC') and without T, Pr, soil water content and air humidity ('- T,ST,Pr,SWC,AH'). The higher a driver is located on the *y*-axis, the more interaction pathways there are between this driver and yield amount. Only the top 25% drivers for each network type are displayed; the full list can be found in SI figure S4.

yield amount (but not necessarily its variability): carbon dioxide, solar radiation, soil salinity, tropospheric ozone concentration, microorganisms (e.g. mycorrhizas), soil temperature, soil pH, soil density, wind and soil nutrient levels. From the management category the following nodes are suggested as important: timing of sowing/harvesting, weed management, irrigation, soil management and drought resistance support. Figure 4 shows the relative ranking of drivers (only top 25%): the *x*-axis contains the four network types (full and three reduced variants) and the *y*-axis the number of interactions up to a path length of four (log-scale). The more interactions a factor controls, the more important it is assumed for yield formation. The results are similar for all three crops, although the relative importance can be crop-specific (SI figure S7). Different thresholds for maximum path lengths do not change the results qualitatively (SI figure S4).

3.2.1. Filtering drivers with low short-term variability

Only factors that are variable in nature can be drivers of variable yields. Therefore, to exclude unlikely drivers of variability, we determine the variation of each factor that is regarded as yield-influencing from our network. Table 1 lists the variability of each factor and whether it is considered in this review. The management options listed above are 'variable' by definition since the farmer can decide at any point in time to apply irrigation, drought support (seed priming only before the growing season), weed control or different soil management options (before and within season). Sowing times can also be highly variable between years, depending on local climatic conditions, cultivar choice, soil parameters and other factors (Craufurd and Wheeler 2009, Portmann *et al* 2010, Waha *et al* 2012, 2013). The impact of management decisions on YV is not assessed here, but should nonetheless be considered in crop models. In the following we only consider environmental variations as source of YV. Interactions between drivers and plant physiological processes are summarized in cursory depth in the next section. An extended and in-depth version with more references can be found in the SI.

3.2.2. Processes affected by water and temperature

The influence of precipitation on yield is paramount in most regions of the globe (Yu *et al* 2014, Ray *et al* 2015), and it is mediated via the SWC. SWC depends on precipitation and other factors like temperature, soil density and management (e.g. tillage) (Leakey *et al* 2009, Hatfield *et al* 2011). The fraction of SWC that is available for uptake by plant roots is further determined by soil salinity or competition (Fuhrer 2003, Tokatlidis 2014). Photosynthesis, temperature regulation, carbon allocation, nutrient uptake and reproduction strongly depend on water to function properly (Boyer and Westgate 2004, Reddy *et al* 2004, Barnabás *et al* 2008, Brouder and Volenec 2008, Farooq *et al* 2009b, Gonzalez-Dugo *et al* 2010, Ahmed *et al* 2013, Jagadish *et al* 2014, Suzuki *et al* 2014). In particular, reproductive processes including anthesis and grain filling are highly sensitive to drought (Acevedo *et al* 2002, Boyer and Westgate 2004, Barnabás *et al* 2008, Lawlor and Tezara 2009, Gonzalez-Dugo *et al* 2010, Thitisaksakul *et al* 2012, Powell *et al* 2012, Ashraf 2014, Farooq *et al* 2014, Jagadish *et al* 2014). Non-optimal water availability

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Table 1. Assessment of the natural variability of important yield-influencing factors in crop growing conditions. The first column contains the factor, the second column its short-term variability in nature (low or high), the third column lists references for the variability, the fourth column contains comments on the factor and the fifth states if the factor is included in this review.

Factor	Variability	References	Comment	Inclusion
Soil water content and precipitation	High	Lobell and Gourdji (2012), Donat *et al* (2013), Ruane *et al* (2015)	SWC buffers Pr variability, but eventually follows the Pr trend (Bell *et al* 2010)	Yes
Temperature (air and soil)	High	Rahmstorf and Coumou (2011), Seneviratne *et al* (2012)	For example influences on yield see Ray *et al* (2015)	Yes
Solar radiation	High	Wang and Dickinson (2013)	Important especially when other factors are not limiting (Tollenaar and Lee 2002, de Bossoreille de Ribou *et al* 2013)	Yes
Tropospheric Ozone	High	Fuhrer (2003), Martiello and Giacchi (2010), Wild *et al* (2012), Tai *et al* (2014), Hoshika *et al* (2015)	Ozone follows temperature, solar radiation and precursor trends nonlinearly McGrath *et al* (2015)	Yes
Wind	High	SI figure S3 for interactions	Aggregate effects are unclear	No
Soil nutrient pools	High	Fageria and Baligar (2005); Porter and Lawlor 1991 (p 173)	Nutrients are key limiting factors for yield (Boote *et al* 2013)	Yes
CO_2	Low	Varotsos *et al* (2007)	Though CO_2 exerts a significant ecophysiological impact on crops (Long *et al* 2006, Leakey *et al* 2009, Sakurai *et al* 2014, Myers *et al* 2014),there is only low within-season variation	No
Soil salinity	Low	George *et al* (1997), Clarke *et al* (2002), Schofield and Kirkby (2003), Lambers *et al* (2008)	Could create variability in yield and production levels at spatially aggregated levels, but only low within-season variation (Ben-Ari and Makowski 2014)	No
Microorganisms	Unknown		May still be instrumental for understanding YV; management influences microorganisms (e.g. Gaudin *et al* 2015)	No
Soil acidity or density	Unknown		No information on its interannual variability is available	No

also has a possibly negative influence on soil micro-organism composition and on the severity of diseases (Hatfield *et al* 2011, Ahmed *et al* 2013).

The yield amount of wheat, maize and rice is reduced with non-optimal temperatures. Early growth, photosynthesis, carbon assimilation, stomatal conductance, plant development and root functioning strongly respond to temperature. This can diminish yields if temperature is too high or low (Schnyder 1993, Acevedo *et al* 2002, Wahid *et al* 2007, Barnabás *et al* 2008, Craufurd and Wheeler 2009, Farooq *et al* 2009a, 2011, Hatfield *et al* 2011, Hasanuzzaman *et al* 2013, Madhu and Hatfield 2013, Jagadish *et al* 2014, Suzuki *et al* 2014). Reproduction, again, is particularly sensitive to temperature extremes (Ishag and Mohamed 1996, Morison and Lawlor 1999, Dupont and Altenbach 2003, Barnabás *et al* 2008, Farooq *et al* 2011, Siebenmorgen *et al* 2013, Jagadish *et al* 2014). Many biochemical processes, like cell respiration and division, leaf senescence or membrane functionality depend on an optimal temperature range (Fuhrer 2003, Wahid *et al* 2007, Farooq *et al* 2009a, Mohammed and Tarpley 2009, Yadav 2010, Farooq *et al* 2011, Hasanuzzaman *et al* 2013, Miura and Furumoto 2013, Jagadish *et al* 2014). High T can also be coupled to an increased O_3 concentration that causes damage on its own (see below).

3.2.3. Processes affected by other important drivers

Solar radiation is the only source of energy for photosynthesis. Radiation is also the ultimate source of all weather variables like temperature. But the relation between radiation and temperature has recently become more complex (Wang and Dickinson 2013), and solar radiation affects crops in additional, distinct ways (Porter and Lawlor 1991 (p 106)). Excess radiation can damage the photosynthetic apparatus or induce oxidative stress, which both reduce the assimilation of C (Reddy *et al* 2004, Lambers *et al* 2008 (p 36)). Low radiation can also limit the uptake of nutrients (Lambers *et al* 2008 (p 268)).

Tropospheric ozone (O_3) is known to cause substantial harm to crops in many regions (Avnery *et al* 2011, McGrath *et al* 2015). Its concentration in the Northern Hemisphere has risen in recent decades, with regional variation (Hoshika *et al* 2015). Increased [O_3] has been shown to enhance leaf senescence, to impair reproductive processes and to lower the resistance against diseases (Fuhrer 2003, 2009, Hatfield *et al* 2011, Beckles and Thitisaksakul 2014). Higher [O_3] can also counterbalance a fertilization effect of CO_2 (Fuhrer 2009, Hatfield *et al* 2011).

Nutrients including nitrogen (N), phosphorus (P) and other micronutrients are essential determinants of crop yield. Their uptake is influenced by temperature, soil characteristics (water content, acidity, salinity), root structure, soil characteristics, weed competition and plant growth (Fuhrer 2003, Barnabás *et al* 2008, Brouder and Volenec 2008, Ahmed *et al* 2013, Ashraf 2014). Nutrients, especially N, and micronutrients like potassium or iron are required for photosynthesis, protein or starch synthesis, stress tolerance, turgor maintenance or ROS scavenging (Porter and Lawlor 1991 (p 13, 39, 55ff.); Hay and Porter 2006 (p 109, 198f); Thitisaksakul *et al* 2012, Powell *et al* 2012, Suzuki *et al* 2014). An excess of nutrients, in contrast, can cause misguided growth or impede grain filling (Schnyder 1993, Yang and Zhang 2006).

3.2.4. Influences on yield quality

Not only yield amount, but also yield quality is variable (e.g. Larcher 1995 (p 289); Dupont and Altenbach 2003, Siebenmorgen *et al* 2013). The assessment described above for yield amount has been performed for yield quality, too. It indicates that essentially the same set of drivers and plant physiological processes is important for the determination of quality (SI figure S6).

3.3. Selecting processes for improving crop models

The drivers of YV identified above affect yields indirectly by their influence on plant physiological processes. With our network we can also identify the relative importance of these processes to guide further development of crop models.

3.3.1. Relative importance of plant physiological processes

The putatively most important processes to transmit variability in growing conditions to YV are those strongly influenced by environmental or management stimuli and at the same time exerting a considerable impact on yields. An ordering diagram is shown in figure 5, which is structured as described in figure 2. Every process is located according to its sensitivity to driver variables on the x-axis and its respective impact on yield levels on the y-axis. We identify the following plant physiological processes as important (located in the top right quadrant): plant growth (split into growth of stem, roots and leaves); the uptake of water and nutrients; photosynthesis; reproduction; stress responses including antioxidant and disease defense; (evapo)transpiration; respiration; cell-internal processes like protein synthesis, turgor maintenance or division; senescence; and stomatal opening regulation. Connections between these processes, their environmental effectors and their influence on yields are found in section 3.2.

Three physiological hierarchy levels of the processes are included in the network: cell level, tissue and whole plant. Processes on the cell level determine those on tissue level (e.g. photosynthesis is required for root growth), and these in turn determine the processes on plant level (e.g. roots define the uptake of water). Growing conditions affect crops on different levels, which is thus reflected in our network.

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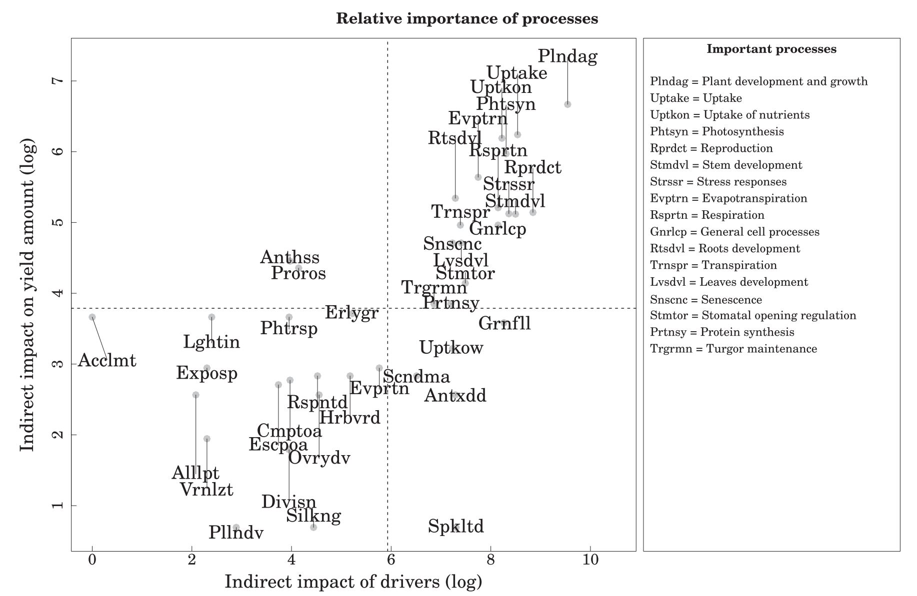

Figure 5. Relative importance of plant physiological processes. Importance is measured by the influence that growing conditions exert on a process (x-axis, log scale) and its respective influence on yield amounts (y-axis, log scale); see methods section for details. The dashed horizontal and vertical lines represent the mean (of the log-ed values) of the x- and y-axis entries, respectively. The processes in the upper right corner are annotated in the legend on the right; these are sorted according to their descending Manhattan distance from the origin (i.e. the sum of x and y location). All other abbreviations are explained in SI table S4. Note that hierarchical levels in the network are flattened, i.e. plant physiological processes can occur both directly and indirectly. For example, stem development ('Stmdvl') is a subcategory of plant development and growth ('Plndag').

There are minor differences between the three crops: wheat exhibits the full set of seventeen processes mentioned above as important, while maize and rice each have three less (senescence, stem development and stomatal opening regulation); SI figure S8. Different thresholds for the maximum allowed interaction path length do not alter the results qualitatively (SI figure S5).

3.3.2. Suggestions for implementing new features in crop models

To support the implementation of new features in crop models we collocate improvement suggestions derived from network structure and importance assessment. We compare the processes identified as important in our network analysis with the status quo of current crop models, as summarized by Boote *et al* (2013). Table 2 compiles this information for each plant physiological process (40 in total, on different hierarchical levels): importance for YV as ranked by the network evaluation (column 2), its implementation priority defined by Boote *et al* (2013) (col. 3), whether important drivers from the growing conditions *directly* influence the process (col. 4–9), and implementation suggestions (last column).

The processes identified as important by our network analysis mostly coincide with the priorities recommended by Boote *et al* (2013). Both sources rank plant growth (in particular roots and leaves plus carbon allocation), reproductive processes including grain filling, the regulation of stomata and canopy energy balance, the nutrient balance, leaf senescence, respiration and photosynthesis (source-sink relationships) as priority for improving crop models. But differences in priority also occur in both directions. We identify cell turgor maintenance and protein synthesis as important, while these are not mentioned in Boote *et al* (2013). These two are usually not resolved in crop models, but rather covered by more coarse processes like water stress response or growth. Boote *et al* (2013), in contrast, rank grain filling, spikelet fertility and the response to pests and diseases as priorities for crop models. Yet we do not find these as primarily important processes in our network analysis. These processes are resolved in our network in the broader categories reproduction and stress responses, which are identified as important. The differences between our network method and the expert-approach by Boote *et al* (2013) are therefore mostly due to the network structure.

Interactions between different processes and the associated literature references for more details, like quantitative thresholds, can be easily extracted from the network. The full network is provided as GraphML source file in the SI for that purpose. Combined interactions between drivers or processes are particularly

Table 2. Plant physiological processes (first column) with their relative importance as our network suggests (c. 2), implementation priority according to our interpretation of Boote *et al* (2013) (c. 3; '1' is high, '2' is medium, and missing is unknown), environmental drivers for each process (only *direct* interactions; c. 4-9) according to our network, and options for improving current implementations (last c.; [B13] means they were also stated in Boote *et al* (2013)). Detailed interactions are listed in the SI. Abbreviations: Pr = Precipitation; SWC = Soil water content; T = Temperature; R_s = Solar radiation; O_3 = Ozone; Nutr = Nutrient levels; SoilT = Soil temperature.

Process	Important (Network)	Priority (Boote *et al* 2013)	Drivers						Improvement options for crop models
			Pr/SWC	T	R_s	[O_3]	Nutr	SoilT	
Plant dev. & growth	Yes	1	x	x	x	x		x	Inclusion of stressors in development timing: water deficit, T [B13] and salinity or O_3
Roots growth	Yes	1	x	x				x	Growth response to edaphic [B13] and weather conditions
Leaves growth	Yes	2	x	x	x			x	Effects of canopy architecture, plant density and supply of nutrients and assimilates [B13]
Stem growth	Yes	2	x	x					Reserve accumulation and utilization under stress (T)
Early growth			x	x	x			x	Interactions of seed quality and stressors (water, T)
Reproduction	Yes	1	x	x	x	x			Fertility effects of high T, higher mechanistic detail [B13]
Grain filling		1	x	x		x	x		Stressors like high T [B13] and O_3; interactions with seed quality
Pollen development		1		x					Effects of high T [B13] and drought
Ovary development		1	x	x					Effects of heat and drought stress
Silking			x	x	x				Effects of heat and drought
Spikelet development			x	x					Effects of high T [B13] and water lack, interactions with elev. CO_2
Anthesis		2	x	x					Effects of high T [B13] and radiation
Stomata regulation	Yes	1	x	x	x	x			Regulation by T, water, CO_2 [B13] and O_3 plus interaction with canopy effects and photosynthesis [B13]
Uptake	Yes								[See subprocess details]
Uptake of water		2	x	x					Interactions with root structure and nutrient uptake
Uptake of nutrients	Yes	1	x	x	x		x	x	Interactions with root structure [B13]; not only N but also P [B13]; effects of saline soils
General cell processes	Yes		x	x					[See subprocess details]
Division			x	x					Effects of drought and hot or cold T
Turgor maintenance	Yes		x	x					Drought and heat effects; interactions with growth and chemical reactions like photosynthesis

Table 2. (Continued.)

Process	Important (Network)	Priority (Boote *et al* 2013)	Drivers						Improvement options for crop models
			Pr/SWC	T	R_s	[O_3]	Nutr	SoilT	
Protein synthesis	Yes			x	x				Impact on yield quality [B13]; effects of high T and radiation
Vernalization				x					Possible reversal under extreme heat
Senescence	Yes	1	x	x		x			Effects of high T [B13], drought, O_3 and excess fertilizer
Evapotranspiration	Yes	1		x	x				[See subprocess details]
Transpiration	Yes	1	x	x	x				Effects of elevated CO_2 and T, connection to photosynthesis [B13], effects of salinity
Evaporation				x	x				[no hints]
Respiration	Yes	2	x	x					Effects of CO_2 [B13] and extreme T
Photosynthesis	Yes	1	x	x	x	x			Scaling up from leaf to canopy or field [B13]; effects of non-optimal T or drought
Light interception									[no hints]
Production of ROS			x	x	x	x			Effects of extreme T and drought, and the impact of ROS on other processes like photosynthesis
Photorespiration			x	x					Effects of heat stress
Acclimation									[no hints]
Stress responses	Yes	2							[See subprocess details]
Antioxidant defense			x	x					Induction by high T or drought through increased ROS production
Sec. metabol. accum.				x					Energy costs by high T
Comp. osmol. accum.			x	x					Energy costs by drought or high T
Expr. of stress prot.				x					Energy costs by high T
Responses to diseases		2		x		x			Incorporation of diseases into crop models [B13]; interaction with energy balance
Escape or avoidance			x						[no hints]
Allelopathy									[no hints]
Herbivory defenses		2							Incorporation into crop models [B13] together with pest models; interaction with energy balance

relevant since plant responses to simultaneous changes in growing conditions often differ from the responses to individual changes (Lobell and Burke 2010, Jagadish *et al* 2014, Ray *et al* 2015). Since extreme events can induce nonlinear responses in crops, their impact on plant physiological processes is of particular importance. These influences are annotated explicitly for the network interactions where mentioned in the associated studies (full network in SI).

4. Discussion

4.1. Validity of the network method

A network structure, derived from literature, is employed to evaluate the importance of growing condition factors and plant physiological processes on YV. Hence it is eminent to have an unbiased knowledge base for its construction. With the systematic approach by pre-defined search terms we aim to keep a literature bias (i.e. the over-representation of aspects like temperature) at a minimum. In addition, all interaction edges have the same weight independent of how often they are confirmed (or contradicted) in the literature, which limits a potential research frequency bias. A strong representation of a process in the literature might, however, reflect its pertinency for implementation. Additionally, a broad literature coverage of aspects like heat or drought stress might stem from its agronomic importance—which further warrants their appropriate consideration in models. Therefore we argue that our findings, which are based on a large interaction network and are robust under different analysis setups, are relevant for crop models.

Our importance assessment does not consider quantitative information in the interactions. But for the relative weighting of process importance a quantitative network would not necessarily be more accurate, as it would introduce more parameters to the method. Furthermore, every quantitative parameter would depend on crop, cultivar and location—which would be beyond the scope of any single meta-study to curtail for 350 interactions. Breeding efforts have achieved higher sensitivities to selected growing conditions, e.g. N and water provision. This trend is neglected in our network, for the same reason of quantitative complexity, but we argue as above that the method would not necessarily benefit from its consideration. Another possible issue that comes with missing quantitative information is that a node with many small influences on other nodes is considered more important than a node with only few but large impacts. Yet many small impacts can also amount to large ones, and the quantity argument goes as above. But if necessary, quantitative information for any specific process can easily be retrieved from the recorded interaction references.

The network unites plant physiological processes on cell, tissue and whole plant level. Single, scale-dependent networks for each of these three would be an alternative approach that respects differences between levels. But we argue that a united approach is justified in our case for three reasons. First, small-scale processes (e.g. cell respiration) accumulate influence over the growing season and therefore can determine yields as much as large-scale processes like, for example, herbivory. Second, the network is constructed to deduce improvement suggestions for crop models, which also need to reflect yield influences on all three levels. Thus we can more easily derive these suggestions with a combined network, but endorse further differentiation in later work. Third, we explicitly aim to capture all relevant mechanisms that may or may not act synchronously to influence yields (synchrony as, for example, in vernalization).

Plant physiological processes can be grouped or aggregated in manifold ways (e.g. Boote *et al* 2013, Bassu *et al* 2014). Our network is therefore only one approach to classify these processes. It is elicited from sequential literature reading of plant physiology text books and independent articles. An assessment of how different basic network structures (differing from figure 3) would affect the results was not tested here. But the network proved flexible enough to incorporate all interactions and elements found in the literature. Some plant responses to growing conditions may not be included in the 350 interactions of our network. Yet we argue that these are likely only minor given the systematic literature mining and the robust driver ranking.

The analysis indicates temperature and precipitation as strong drivers of YV—which is well-known and thus confirms the validity of our method. But we have also identified further factors whose own variability could imply variability in yields. Drivers which our network approach labels as ‘unimportant’ are not necessarily unimportant in reality—the relative weighting applied here only assigns more weight to the others. In contrast, the drivers defined as important by the network structure have only the potential to cause variability. Yet the actual importance depends on the specific combination of the individual components of the growing conditions. Although CO_2 or soil salinity are not regarded as important contributors to YV, they can strongly influence responses to other stressors via interacting effects (Jagadish *et al* 2014). Adequately representing yield quality is equally judged an essential target for crop model improvement, evidenced by the 13 direct influences on yield quality in the network.

The close similarity of results for wheat, maize and rice arises from two independent factors. First, the network edges are often (68%) based on publications that are valid for all three crops considered. Second, the network is qualitative only such that quantitative distinctions between crops are not accessible. Differences between crops (e.g. rice is usually irrigated, maize is a C_4

crop, winter wheat requires vernalization) are not questioned. But with regard to modeling the generality of the drivers identified is beneficial, since most of the mechanistic pathways are shared between crops.

The network essentially reflects the complexity of plant regulatory systems. This entails a high 'importance' for drivers or processes that are involved in several regulatory pathways, i.e. importance reflects complexity. Complex systems may either be prone to abrupt state changes under disturbances (Robbirt *et al* 2014, Willmer 2014, Zscheischler *et al* 2014, Franklin *et al* 2016) or enhance the stability of a system (an example is resilience from biodiversity). The current network does not reveal whether a process that influences YV actually enhances or dampens it. This requires deeper inspection of each single interaction with quantitative information. Our method suggests exactly these crucial points that need further inspection. One possible inspection approach is a recursive refinement of the network into single-process subsets.

4.2. Applicability of the implementation suggestions

Although the network has been constructed without input from crop models we apply it to guide model improvement strategies. This approach is uncommon, but we adopted it for maintaining an 'outside' look on the models inspired by experimental literature alone. In addition the very diverse types and characteristics of models (Rosenzweig *et al* 2014, Elliott *et al* 2015) require an abstract approach that does not depend on a certain class of models. The agreement about the major improvement points between our network method and the expert approach by Boote *et al* (2013) show the efficacy of the network method to detect essential features from the literature. It also justifies the assumption that 'importance' can be derived from the number of connections in the network. Differences in priorities reflect the potential for supplementing one approach with the other.

Many of the process improvement options for crop models are targeting currently less well represented physiological interactions. These general suggestions have to be adjusted for each particular model. There is no guarantee that a crop model eventually becomes better in modeling yield (variability) with a finer resolution of processes or by adding new ones. More processes require more parameters, which could entail model or calibration errors. The necessary experimental data are not easy to find, but one possible starting point is the AgTrials database[4]. Some processes may not yet be implemented for their high complexity paired with unclear benefits for the model. Examples are the crop responses to pests and diseases (high specificity of crop–pathogen–environment interaction; Luck *et al* 2011) or to an elevated ozone concentration (lack of global databases, unclear effect on aggregate level). Nonetheless these have potential to help understanding of YV in diverse environments, and from sources other than temperature or precipitation. Regional-scale crop patterns have been studied as causes of YV by Ben-Ari and Makowski (2014), and genetic traits in YV by Mickelbart *et al* (2015). The focus on plant physiological process level in our analysis complements these two approaches.

5. Conclusion

We have applied a novel methodology for a systematic literature review to identify and rank the importance of drivers and plant physiological processes for crop YV. We have also derived a comprehensive list of target points for improving crop models with respect to YV. As expected, our method confirms that current modeling approaches have addressed many of the important drivers of YV. Thus our approach can be seen as a cross-validation of existing modeling concepts. However, we also show that the drivers and the mechanisms implemented are not sufficiently comprehensive, which thus can guide future model improvement. Our network is a unique structured summary of the literature and its free accessibility can support the improved representation of YV in crop models. In particular the network interaction structure and the rich quantitative literature information associated with it can serve as a starting point.

The approach could be extended by a semi-automatic text mining, extracting the most relevant information from literature databases. Text mining has successfully been applied in medical bioinformatics (Zhu *et al* 2013, Fluck and Hofmann-Apitius 2014, Fleuren and Alkema 2015). Our network-based review could serve as a first step towards this. We have shown its methodical validity as a structured, consistent and scalable dictionary of literature knowledge. The approach is easily applicable to many other fields of research.

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2.2 Supplementary Information

The supplementary information is printed in scaled form since its original version is also available with the online version of the article.

Contents

This supplementary material contains additional information on the article "A network-based approach for semi-quantitative knowledge mining and its application to yield variability". Please refer to the main text for descriptions and context.
Its order is as follows: supplementary text on interactions between growing conditions and plant physiological processes, figure descriptions, figures, table descriptions and tables.

Supplementary text

Detailed interaction descriptions between growing conditions and plant physiological processes

This section contains the extended versions of the short interaction descriptions in section 3.2, in particular with the references for all interactions.

Processes affected by precipitation and soil water content

Precipitation is a major climatic determinant of yield (Yu et al., 2014). This influence is usually mediated via the soil water content (SWC), which depends on several factors: precipitation, evapotranspiration, temperature, soil density and texture, CO_2 concentration, soil management like the choice of tillage method and irrigation (Porter and Lawlor, 1991[p.230f]; Larcher, 1995[p.224]; Farooq et al., 2014; Hatfield et al., 2011; Leakey et al., 2009). The fraction of SWC that is available for uptake by plant roots is further determined by soil salinity, temperature or competition (Fuhrer, 2003; Tokatlidis, 2014; Larcher, 1995[p.379]). The available water is of paramount importance for manifold plant physiological processes for all three crops.

Photosynthesis strongly depends on water to function properly: under drought the leaf area recoils, the stomata close to diminish transpirational loss, leading to less CO_2 influx, Rubisco and other enzymes are downregulated and more reactive oxygen species (ROS) are produced which attack, among others, cell membranes. Reduced carbon (C) assimilation rates are the consequence (Barnabás et al., 2008; Farooq et al., 2009a; Jagadish et al., 2014; Lawlor and Tezara, 2009; Lopes et al., 2011; Reddy et al., 2004; Suzuki et al., 2014).

Too low water availability leads to retarded **growth**, evidenced by reduced height or tillering (Jagadish et al., 2014; Reddy et al., 2004; Suzuki et al., 2014), smaller leaves (Acevedo et al., 2002; Hay and Porter, 2006[p.45f]; Lambers et al., 2008[p.347]), impaired cell division (Barnabás et al., 2008; Boyer and Westgate, 2004; Farooq et al., 2009a), reduced cell turgor (Larcher, 1995[p.384]; Farooq et al., 2009a; Reddy et al., 2004) or delayed wheat germination and emergence (Acevedo et al., 2002). Roots, however, grow longer under drought conditions to tap further water reserves in the soil (Reddy et al., 2004; Lambers et al., 2008[p.348f]; Farooq et al., 2009a). Water-logging, i.e. low-oxygen conditions due to excess water, can also trigger adverse effects on root and shoot in wheat and maize (Ashraf, 2014; Hossain and Uddin, 2011). The uptake of nutrients can be lower under dry conditions due to three reasons: less mobility in the soil, less inflow into roots due to reduced water inflow and disturbance of the uptake processes within the plant (Porter and Lawlor, 1991[p.230]; Hay and Porter, 2006[p.105]; Lambers et al., 2008[p.261]; Ashraf, 2014; Barnabás et al., 2008; Brouder and Volenec, 2008; Farooq et al., 2009a; Gonzalez-Dugo et al., 2010). Water-logging can equally reduce the uptake of nutrients, partly due to leaching (Porter and Lawlor, 1991[p.231]; Ahmed et al., 2013).

Reproductive processes are highly sensitive to drought: sterility or kernel abortion rates increase (Boyer and Westgate, 2004; Farooq et al., 2014; Jagadish et al., 2014), anthesis in wheat or maize is delayed (Hay and Porter, 2006[p.25]; Farooq et al., 2014), spikelet development in wheat is impaired (Acevedo et al., 2002) and silking in maize is delayed and asynchronous (Hay and Porter, 2006[p.25]; Barnabás et al., 2008; Farooq et al., 2009a). The fertilization of ovaries is particularly susceptible to drought in rice (Barnabás et al., 2008). Grain filling – the synthesis and transport of starch and protein to the kernels – is sensitive to lack of water: a lower grain weight and kernel number can be induced (Ashraf, 2014; Jagadish et al., 2014), the starch synthesis is inhibited, leading to a higher protein content in the grains and a changed starch composition (Hay and Porter, 2006[p.208]; Ashraf, 2014; Beckles and Thitisaksakul, 2014; Thitisaksakul et al., 2012), and the duration is reduced (to some extent counter-balanced by an increased filling rate) under drought in rice (Farooq et al., 2009a). Water-logging also leads to lower grain numbers and grain weight in wheat (Ashraf, 2014; Powell et al., 2012).

The conductivity of the **stomata** (cavernous openings on the underside of leaves which serve to let in CO_2 for photosynthesis, to dispose of unnecessary O_2 and also to regulate temperature and water demand through transpiration; Larcher, 1995[p.83] and Fuhrer, 2009) is decreased at a low SWC, leading to less CO_2 influx and possibly to higher canopy and leaf temperatures (Larcher, 1995[p.385]; Morison and Lawlor, 1999; Lambers et al., 2008[p.54]; Farooq et al., 2009a; Fuhrer, 2009; Jagadish et al., 2014; Lawlor and Tezara, 2009; Lopes et al., 2011), which can impair photosynthetic C assimilation. Water lack or excess can disturb **respiration** processes in shoot or root (Larcher, 1995[p.375ff]; Lambers et al., 2008[p.199,p.355f]), which thus provide less energy for growth or yield development. **Senescence** of leaves is accelerated under drought or water-logging, leaving less photosynthates available for grain filling (Ahmed et al., 2013; Farooq et al., 2014; Gonzalez-Dugo et al., 2010; Jagadish et al., 2014). The production of ROS increases under drought, in particular with high light, and their balance with antioxidants is disturbed. This causes an energy-depriving **oxidative stress** for the plant (Ashraf, 2014; Farooq et al., 2009a; Farooq et al., 2014; Lawlor and Tezara, 2009; Reddy et al., 2004). Water lack can trigger the accumulation of compatible osmolytes to compensate osmotic stress (Farooq et al., 2014; Reddy et al., 2004). Non-optimal water availability also has a possibly negative influence on soil **microorganism composition** (Ahmed et al., 2013; Hatfield et al., 2011) and on the severity of **diseases**, but the direction of change depends on individual plant-pathogen-environment factors (Luck et al., 2011).

Processes affected by temperature of air and soil

An extensive body of literature identifies temperature as one of the most important effectors on plant physiological processes and yields. Wheat, maize and rice all exhibit negative responses of yield amount to elevated (beyond optimum) T, evidenced by lowered grain numbers or grain mass (Hatfield et al., 2011; Jagadish et al., 2014; Wahid et al., 2007). Rice seems to be affected in particular by increased nighttime T (Siebenmorgen et al., 2013). Yield quality (protein composition and starch content) is equally changed with heat stress, possibly inducing a lower baking quality in wheat (Dupont and Altenbach, 2003).

Air T influences **soil temperature** (Porter and Lawlor, 1991[p.165f]), which is a key determinant of the early growth phases of crops (Hay and Walker, 1989[p.11]; Hay and Porter, 2006[p.40]; Farooq et al., 2009b). Both too low or too high soil T can cause a failure of plant establishment (Porter and Lawlor, 1991[p.230]; Acevedo et al., 2002; Farooq et al., 2009b) and limit the water available to roots (Larcher, 1995[p.379]; Farooq et al., 2009b; Lobell et al., 2013).

Increased air T facilitates the spreading of **diseases** (Suzuki et al., 2014) or alters their severity (Luck et al., 2011). Herbivory insect ecology is also linked to T (Hatfield et al., 2011; Luck et al., 2011). The **growing season** is shorter with higher T, as the required growing degree days for phenology transitions are acquired faster, which leads to fewer spikelets e.g. in wheat (Barnabás et al., 2008) and also less solar radiation intercepted (Hatfield et al., 2011).

An additional problem that could come along with high T is an increased O_3 concentration that causes damage on its own (see Fuhrer (2003) and below).

Temperature exerts a strongly regulating influence on almost all biochemical processes, including **photosynthesis**: an intermediate range is optimum for C assimilation (Farquhar et al., 1980), but extremes at both ends can severely confine the ability of plants to acquire C in all three crops: the activity of Rubisco – the major photosynthesis enzyme – and the chlorophyll content decrease with high T (Barnabás et al., 2008; Farooq et al., 2011; Hasanuzzaman et al., 2013; Hatfield et al., 2011; Wahid et al., 2007). Heat stress can also induce an increased production of ROS, which require energy to be scavenged that is therefore not available for growth (Farooq et al., 2011; Hasanuzzaman et al., 2013; Jagadish et al., 2014; Wahid et al., 2007). A raised propensity of Rubisco to ligate with O_2 instead of CO_2 – triggering the so-called photorespiration, a process which requires energy to cover up for the unwanted reaction with O_2 – further depresses the C assimilation under elevated T (Hay and Walker, 1989[p.55]; de Bossoreille de Ribou et al., 2013; Farooq et al., 2011; Fuhrer, 2003). Too low T exerts comparable effects: the production of ROS is increased (Farooq et al., 2009b), free oxygen radicals can accumulate even with slightly increased radiation (Lambers et al., 2008[p.239]; Miura and Furumoto, 2013), the circadian regulation can be disturbed in maize (Farooq et al., 2009b) and the chemical reaction processes become slower in general (Larcher, 1995[p.108f.]; Acevedo et al., 2002; Farooq et al., 2009b; Suzuki et al., 2014).

The **stomatal** regulation is closely connected with photosynthesis. Raised T exerts a contradictory influence on the conductivity: surging transpiration needs for cooling would lead to an increased conductivity (Porter and Lawlor, 1991[p.231]; Larcher, 1995[p.239]; Hatfield et al., 2011), but a high vapor pressure deficit (VPD), which rises with T and decreasing SWC, would lead to a closing of stomata to preserve water reserves (Lambers et al., 2008[p.54]; Fuhrer, 2009; Hasanuzzaman et al., 2013; Lobell and Gourdji, 2012; Suzuki et al., 2014) and therefore mingles with the former stimulus. A reduced stomatal conductance allows less CO_2 to enter and traps O_2 inside, thereby reducing photosynthetic efficiency (Larcher, 1995[p.78]). The stomata response options to high T are therefore co-regulated to optimize between all these incentives.

Plant development is largely influenced by T (Porter and Lawlor, 1991[p.23]; Larcher, 1995[p.279ff]; Hay and Porter, 2006[p.9]; Craufurd and Wheeler, 2009), in particular by extremes. Higher T leads to faster development with impaired growth (Jagadish et al., 2014). Intense heat negatively affects the early growth phases in wheat and rice (Hasanuzzaman et al., 2013), reduces the leaf size in wheat and maize to lower the water requirements for transpirational cooling (Acevedo et al., 2002; Farooq et al., 2009b; Hasanuzzaman et al., 2013) and severely impedes the root functioning in wheat and maize (Lambers et al., 2008[p.346]; Farooq et al., 2009b; Farooq et al., 2011; Madhu and Hatfield, 2013). Vernalization in winter wheat is possibly reversed under high T (Rötter and Van De Geijn, 1999). Chilling T can impede root growth (Porter and Lawlor, 1991[p.230]), early growth and leaf development in maize (Farooq et al., 2009b) or stem reserve accumulation in wheat (Schnyder, 1993).

Virtually all **reproductive processes** in the three cereals are impinged by T extremes. Both too cold or high T might cause pollen or spikelet sterility (Boyer and Westgate, 2004; Morison and Lawlor, 1999; Rötter and Van De Geijn, 1999; Lambers et al., 2008[p.242]; Barnabás et al., 2008; Boote et al., 2013; Farooq et al., 2011; Hasanuzzaman et al., 2013; Hatfield et al., 2011; Luo, 2011; Powell et al., 2012; Yadav, 2010). Heat stress can cause misregulations on several reproductive processes, including kernel abortion (Ashraf, 2014; Barnabás et al., 2008; Jagadish et al., 2014) or the asynchrony of silking and fertilization time in maize (Barnabás et al., 2008). The process of **grain filling** is especially sensitive to heat stress. Increased T affects its duration (shorter) and rate (higher) in cereals, with unclear results: both effects could balance, but if T, in particular the daily minimum, rises strongly the negative effect of the shorter duration dominates (Barnabás et al., 2008; Dupont and Altenbach, 2003; Farooq et al., 2011; Hasanuzzaman et al., 2013; Hatfield et al., 2011; Ishag and Mohamed, 1996; Jagadish et al., 2014; Siebenmorgen et al., 2013). The grain composition is altered by too high T: both the starch and protein synthesis and deposition are affected, with the starch remobilization and composition reacting more pronouncedly. This induces a lowered starch-to-protein relation and a changed chemical composition of both ingredients (Blum, 1998; Hay and Porter, 2006[p.208]; Ashraf, 2014; Barnabás et al., 2008; Beckles and Thitisaksakul, 2014; Farooq et al., 2011; Jagadish et al., 2014; Thitisaksakul et al., 2012). This could, for example, alter the baking quality of bread wheat (Dupont and Altenbach, 2003; Wahid et al., 2007). Furthermore, grain size could be depressed by heat stress (Hasanuzzaman et al., 2013; Hatfield et al., 2011; Sánchez et al., 2014).

On the **cell level** effects of too high or too low T include a higher respiration rate (Larcher, 1995[p.106f]; Hay and Porter, 2006[p.141]; Lambers et al., 2008[p.127f]; Hasanuzzaman et al., 2013) which could decrease yields especially in rice (Mohammed and Tarpley, 2009), a hastened leaf senescence (Hay and Walker, 1989[p.17]; Jagadish et al., 2014) and a lowered nutrient uptake at chilling T (Lambers et al., 2008[p.268]). Cell turgor could be weakened and cell division impaired with heat or cold stress, leading to retarded growth (Farooq et al., 2009a; Farooq et al., 2009b; Hasanuzzaman et al., 2013). Protein functionality and synthesis is dependent on an optimal T range (Porter and Lawlor, 1991[p.17]; Miura and Furumoto, 2013; Wahid et al., 2007), similar to the cell membrane which can become dysfunctional under extremes at both ends (Larcher, 1995[p.340]; Yadav, 2010).

Finally, T simultaneously induces and impacts on **stress responses** of crops: the resistance to diseases (Fuhrer, 2003) or the antioxidant defense (Farooq et al., 2011; Hasanuzzaman et al., 2013) are necessary during heat stress, but can also be impaired by it. Above-optimum T can trigger the accumulation of compatible osmolytes or secondary metabolites, which requires energy (Hasanuzzaman et al., 2013; Wahid et al., 2007).

Processes affected by solar radiation

Solar radiation is the only source of energy for photosynthesis and all subsequent processes. Radiation is also the ultimate source of all weather variables like temperature. But the relation between radiation and temperature has recently become more complex (Wang and Dickinson, 2013), and solar radiation affects crops in additional, distinct ways. Excess radiation can induce damage on the photosynthetic apparatus, persistently reducing the assimilation of C through "photo-inhibition" (Larcher, 1995[p.334]; Lambers et al., 2008[p.36]). An increased ROS production can occur at high light inception, especially in times of drought (Reddy et al., 2004). Plant development and reproduction is partly controlled by radiation (Larcher, 1995[p.279ff]), also in the germination stage (Lambers et al., 2008[p.380]). Under optimal conditions the leaf area of plants is adjusted to the available amount of light (Lambers et al., 2008[p.341]) and its development needs to match with the season to avoid a waste of energy (too much investment into a large leaf area) or light (too small leaf area) (Hay and Walker, 1989[p.21f]; Hay and Porter, 2006[p.59]). Shading in maize plants can increase the anthesis-to-silking interval and thus lead to a lower grain set (Hay and Porter, 2006[p.25]).

In the presence of ample nutrient supply low radiation can limit their uptake (Lambers et al., 2008[p.268]). Radiation also has an influence on protein synthesis (Porter and Lawlor, 1991[p.19]) and determines the microclimate temperature perceived by the plant (Hall et al., 1993[p.48]). A direct linear increase in accumulated biomass with cumulative solar radiation in the absence of stresses (Porter and Lawlor, 1991[p.106]) underlines the salient importance of radiation.

Processes affected by tropospheric ozone

Tropospheric ozone (O_3) is known to cause harm to crops in many regions of the world (Booker et al., 2009; Fuhrer, 2003; Wilkinson et al., 2012), estimated to a global yield loss of about 4-10% for wheat and maize (Avnery et al., 2011). Its concentration in the Northern Hemisphere has risen strongly in recent decades (Hoshika et al., 2015).

Increased [O_3] has been shown to enhance leaf senescence (Hay and Porter, 2006[p.116]), to increase ROS production (Fuhrer, 2009), decrease photosynthesis rates in rice and wheat (Hay and Porter, 2006[p.115]; Hatfield et al., 2011), and to counterbalance the positive effects of CO_2 on yield amount (Fuhrer, 2009). This questions the fertilization effect of CO_2 when temperature, CO_2 and O_3 rise simultaneously (Booker et al., 2009; Fuhrer, 2003).

Reproductive processes can be inhibited by high levels of ozone, especially in the grain filling phase whose duration is decreased by enhanced leaf senescence (Fuhrer, 2009). The starch composition and functionality can be altered by raised ozone levels, leading to a reduced N use efficiency in grains (Beckles and Thitisaksakul, 2014; Fuhrer, 2003). Higher O_3 induces a raised protein content in grains, but at the price of a reduced yield amount (Fuhrer, 2003).

Finally, ozone levels exert an influence also on weeds, usually equally detrimental for them. The occurrence and severity of pests and diseases changes with O_3, but directions are equivocal and interactions complex (Fuhrer, 2009). Thus no simple conclusion for yield levels can be drawn. The resistance of plants to diseases, though, can be lowered with increased O_3 (Fuhrer, 2003).

Processes affected by soil nutrient pools

Nutrients - including nitrogen (N), phosphorus (P) and other micronutrients - are essential determinants of yield levels. Two process categories are related to nutrients: the uptake via the roots and the effects of nutrients in the plant.

The **uptake** of nutrients is influenced by temperature, soil water content, root structure, plant growth and soil characteristics. Low T lowers the uptake, and soil T is a primary determinant of nutrient availability to the roots (Lambers et al., 2008[p.268], Brouder and Volenec (2008)). A low SWC severely limits the uptake of nutrients by reducing their solubility in soil (Ashraf, 2014; Barnabás et al., 2008; Brouder and Volenec, 2008; Farooq et al., 2009a; Gonzalez-Dugo et al., 2010), and also by reducing transpiration and thus the flow of water through the plant that carries nutrients (Brouder and Volenec, 2008). Excess water, in contrast, can lead to nutrient leaching (Porter and Lawlor, 1991[p.231]) and reduced uptake (Ahmed et al., 2013). The root structure controls nutrient uptake: larger surface, symbiosis with mycorrhizas and deeper branching allow the uptake of more nutrients (Porter and Lawlor, 1991[p.142ff], Lambers et al., 2008[p.413], Brouder and Volenec (2008)). The growth rate of the plant determines the uptake of N (Hay and Porter, 2006[p.195f], Lambers et al., 2008[p.346f]). The uptake of nutrients into cells also depends on the available photosynthates since this process requires energy (Lambers et al., 2008[p.265], Porter and Lawlor, 1991[p.104]). A high soil salinity or a low pH can both reduce the nutrient uptake (Larcher, 1995[p.398], Lambers et al., 2008[p.257]). Another factor that impacts on nutrient availability for the crop is weed competition (Fuhrer, 2003).

Once the nutrients are taken up by the plant they influence **several mechanisms**. The photosynthesis rate critically depends on an optimum supply of nutrients, in particular N (Hay and Walker, 1989[p.76ff]; Porter and Lawlor, 1991[p.7f]; Lambers et al., 2008[p.58]) for radiation interception (Hay and Porter, 2006[p.109,198f]) and iron for the light reaction (Porter and Lawlor, 1991[p.55ff]). Respiration rates in the shoot decrease (Lambers et al., 2008[p.123]), but increase in roots under low nutrient supply to stimulate tapping of further nutrient reserves (Porter and Lawlor, 1991[p.104,125f]; Hay and Porter, 2006[p.120]; Lambers et al., 2008[p.351]).

Lowered photosynthesis and changing respiration patterns lead to a retarded shoot growth under nutrient (N, P) limitation. This includes leaves (Hay and Walker, 1989[p.18]; Acevedo et al. (2002); Hay and Porter, 2006[p.53]; Lambers et al., 2008[p.349ff]), wheat tillers (Hay and Walker, 1989[p.179f]) and spikelets (Acevedo et al., 2002), and the whole organism (Porter and Lawlor, 1991[p.16,68ff]; Lambers et al., 2008[p.322f]). Nutrients, especially N, are required for protein synthesis (Porter and Lawlor, 1991[p.13]), starch synthesis (Thitisaksakul et al., 2012), secondary metabolites (Porter and Lawlor, 1991[p.91]) or stress tolerance in rice (Powell et al., 2012). Micronutrients such as potassium are essential for turgor maintenance (Porter and Lawlor, 1991[p.39]), amino acid synthesis (Porter and Lawlor, 1991[p.15]), ROS scavenging (Suzuki et al., 2014) or leaf longevity (Hay and Walker, 1989[p.17]).

In contrast an excess of nutrients, N in particular, can cause misguided growth (Hay and Walker, 1989[p.175]; Larcher, 1995[p.188]) or delay senescence and thereby impede grain filling (Schnyder, 1993; Yang and Zhang, 2006).

Supplementary figures

Regions with yield variation, but not from temperature or precipitation

Ray et al. (2015) have performed an extensive correlation of yields with temperature and precipitation variables across the globe. On average they can explain one third of YV by weather variation, but with large differences between regions. Some of the actual weather-induced variation in yields might be lost in the aggregation procedure. But nonetheless there are several regions on the globe with substantial variability in yields (i.e. coefficient of variation > 0.15) where any tested combination of T and Pr can explain only less than half of it (i.e. $R^2 < 0.45$). Examples for these regions include large parts of Russia, the US, India, Argentina, Australia and the Middle East (for wheat), hundreds of counties in the US, substantial parts of Mexico, Brazil, Argentina, India, Russia, South East Europe, Ecuador, Ethiopia and the whole of Tanzania (for maize), and parts of Brazil, India, China and Western Africa (for rice). These regions sum up to 18%, 39% and 42% of the planted regions for wheat, maize and rice, respectively. A map of these regions for wheat, maize and rice is shown in Figure S1.

Network

The network terminology used in the paper is described with an example graph in Figure S2. The network constructed from the literature and used in our further analysis is shown in Figure S3. The source file is available in GraphML format, which can be read by different open source graph software packages (e.g. yEd). The six edges added without explicit literature reference are tagged with "personal communication" in the network.

Results for different maximum path lengths

The relative importance of environmental drivers for the determination of yield amount, for different maximum path lengths, is shown in Figure S4. Similarly the relative importance of plant processes, split by different allowed maximum path lengths through the network, is pictured in Figure S5.

Analysis for yield quality

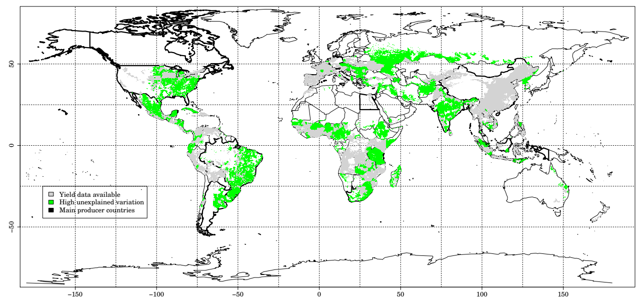
The relative importance of environmental drivers for the determination of yield **quality** is shown in Figure S6.

Driver importance split by crops

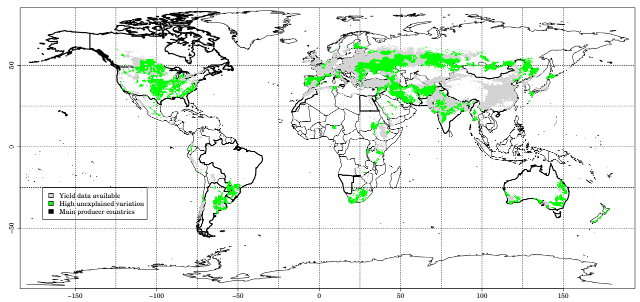
The relative importance of environmental drivers for determination of yield amount, split by crops, can be seen in Figure S7.

Process importance split by crops

The relative importance of physiological processes for determination of yield amount, split by crops, can be seen in Figure S8.

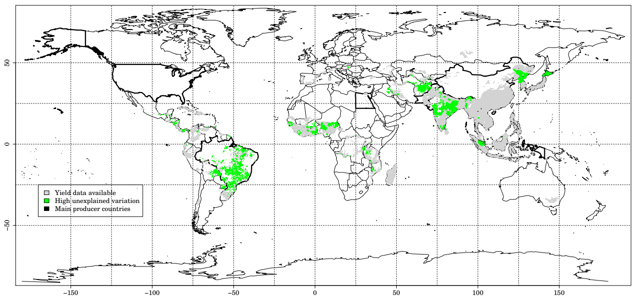


(a) Maize



(b) Wheat

Figure S1: [continued on next page]



(c) Rice

Figure S1: Regions where yield variability is substantial, but less than half due to weather variation. Panel (a) shows maize, (b) wheat and (c) rice. Variation and explanatory power of weather are taken from Ray et al. (2015). Countries with bold outlines are main producers for the respective crop. Regions marked in grey have data, and regions marked in green have a substantial yield variability (CV > 0.15), but weather variation can explain less than half of it ($R^2 < 0.45$). For more details please refer to Ray et al. (2015).

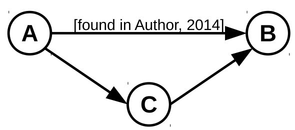


Figure S2: Example for the network terminology used throughout the paper. A, B and C are *nodes*, and the connections between them are *edges* (interactions), such that network $N = (V, E) = (\{A, B, C\}, \{e_1 : A \to B,\ e_2 : A \to C,\ e_3 : C \to B\})$. Possible paths from A (*source node*) to B (*target node*) comprise the direct one $q_1 = e_1$ (length $|q_1| = 1$) and the indirect one $q_2 : e_2 + e_3$, with $|q_2| = 2$. The *degree* of all nodes is 2, but with different compositions: A has in-degree 0 and out-degree 2, while B and C have in-degrees of 2 and 1, and out-degrees of 0 and 1, respectively. Each edge can be labeled as indicated for $A \to B$. The *impact* of A on B with a maximum path length of 1 is 1, and with a maximum length of 2 it is 2 (two paths with at most length 2 exist between A and B).

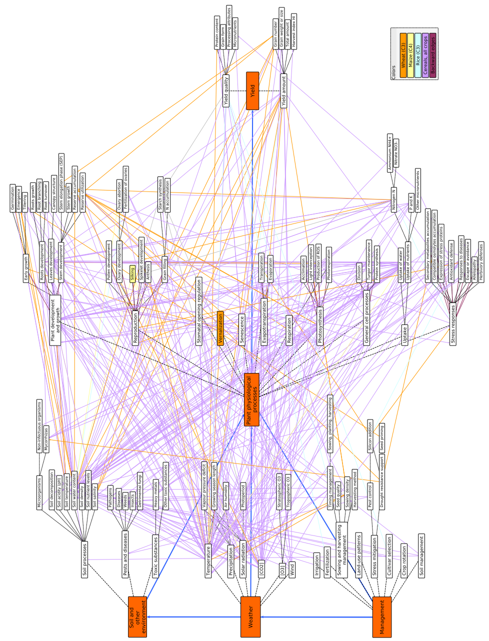


Figure S3: The full network, containing 130 nodes and 509 edges, of which 350 are interactions between nodes. The figure is zoomable such that the labels are legible, and the corresponding GraphML source file is provided. The five top categories 'Weather', 'Soil and other environment', 'Management', 'Plant physiological processes' and 'Yield' are represented by the five thick red boxes; these are split into sub- and subsubcategories by dashed lines. Interaction edges can have one of five colors (see box in bottom right part): brown for edges that are only valid for wheat, yellow for maize, blue for rice, magenta for all crops and dark purple for backward edges from subsubcategories to subcategories (which are necessary to avoid dead ends). Edge labels were dropped for better display, but can be found in the GraphML source file.

Supplementary tables

Network

Network figures for each crop are shown in Table S1.

Study selection

The original keyword list devised for the systematic search can be found in Table S3. The studies selected from the literature with the help of these keywords and used to construct the interaction network are listed in Table S2.

A few notes on the filtering of search results: book chapters were excluded (as six textbooks were used for the initial network construction, and afterwards the search was more focused on variability or unusual interactions); if two very similar reviews were available (i.e. same author and same topic) only the later one was selected; many papers with 'yield' in its topic are not related to agriculture at all (e.g. metallurgy); the six text books and two papers were added manually (Acevedo (2002) for its general overview of wheat development and Leakey (2009) for its general description of CO_2 effects); search terms were augmented by "plant" if more than 1,000 results appeared for the 'Topic + DT=Review' search. Also note that papers which were not selected from the vast amount of literature are not necessarily unimportant; but we argue that the overall structure of the network, and the results are robust against the omission of a few studies. An even more unbiased alternative to this manual selection could be a text-mining approach (see Conclusions section in main paper).

Abbreviations

The six-letter abbreviations used in all figures throughout the paper are listed in Table S4, together with their full meaning.

Table S1: Network statistics, separated by crop types. An exclusive node for wheat is 'Vernalization', and for maize 'Silking'; rice has none. The total number of edges represents the number of edges without those that contain no reference to the desired crop, and the unique edges are those which exist only for the desired crop. Average node degree is number of total edges divided by number of nodes. For the number of edge labels all annotations with the desired crop were counted.

Crop	# Nodes	# Total edges	# Unique edges	Av. node degree	# Edge labels
All	130	509	159	3.92	363
Wheat	129	494	43	3.83	105
Maize	129	454	7	3.52	36
Rice	128	458	8	3.58	32

Table S2: Articles and text books selected for the network constructions. The studies were selected from the Web of Knowledge between May 2014 and January 2015 and are the result of an extensive filtering step from approx. 460,000 initial search results down to 60.

Nr	Author	Year	Title	Journal	Search term
1	Acevedo, E. et al.	2002	Wheat growth and physiology	FAO Publication	selected manually
2	Ahmed, F. et al.	2013	Water-logging Tolerance of Crops: Breeding, Mechanism of Tolerance, Molecular Approaches, and Future Prospects	Biomed Research International	Water Logging Yield (Topic + Review)
3	Altenbach, S. et al.	2012	New insights into the effects of high temperature, drought and post-anthesis fertilizer on wheat grain development	Journal of Cereal Science	Yield Climate Wheat (Topic + Review)

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Table S2 – continued from previous page

Nr	Author	Year	Title	Journal	Search term
4	Ashraf, M. et al.	2014	Stress-Induced Changes in Wheat Grain Composition and Quality	Critical Reviews in Food Science and Nutrition	Temperature Wheat Yield (Topic + Review)
5	Barnabas, B. et al.	2008	The effect of drought and heat stress on reproductive processes in cereals	Plant, Cell & Environment	Temperature Wheat Yield (Topic + Review)
6	Beckles, D. et al.	2014	How environmental stress affects starch composition and functionality in cereal endosperm	Starch	Yield Stability Maize (Topic + Review)
7	Blum, A.	1998	Improving wheat grain filling under stress by stem reserve mobilization	Euphytica	cited by (Barnabas 2008)
8	Boote, K. et al.	2013	Putting mechanisms into crop production models	Plant, Cell & Environment	Yield Climate Maize (Topic + Review)
9	Boyer, J. et al.	2004	Grain yields with limited water	Journal of Experimental Botany	cited by (Barnabas 2008)
10	Brouder, S. et al.	2008	Impact of climate change on crop nutrient and water use efficiencies.	Physiologia Plantarum	Yield Climate Rice (Title)
11	Cairns, J. et al.	2011	Influence of the soil physical environment on rice (Oryza sativa L.) response to drought stress and its implications for drought research	Field Crops Research	Yield Variability Rice (Topic + Review)
12	Craufurd, P. et al.	2009	Climate change and the flowering time of annual crops.	Journal of Experimental Botany	Yield Variability Wheat (Topic + Review)
13	De Bossoreille de Ribou, S. et al.	2013	Plant science and agricultural productivity: why are we hitting the yield ceiling?	Plant Science	Water Rice Yield (Topic + Review)
14	Dolferus, R. et al.	2011	Abiotic stress and control of grain number in cereals.	Plant Science	Temperature Wheat Yield (Topic + Review)
15	Dupont, F. et al.	2003	Molecular and biochemical impacts of environmental factors on wheat grain development and protein synthesis	Journal of Cereal Science	Temperature Wheat Yield (Topic + Review)
16	Farooq, M. et al.	2009	Plant drought stress: effects, mechanisms and management	Agronomy for Sustainable Development	Drought Yield (Topic + Review)
17	Farooq, M. et al.	2009	Chilling tolerance in maize: agronomic and physiological approaches	Crop & Pasture Science	citing (Farooq 2009a)
18	Farooq, M. et al.	2011	Heat Stress in Wheat during Reproductive and Grain-Filling Phases	Critical Reviews in Plant Sciences	Yield Stability Wheat (Topic + Review)
19	Farooq, M. et al.	2014	Drought Stress in Wheat during Flowering and Grain-filling Periods	Critical Reviews in Plant Sciences	Drought Yield (Topic + Review)
20	Fuhrer, J.	2003	Agroecosystem responses to combinations of elevated CO2, ozone, and global climate change	Agriculture, Ecosystems & Environment	Yield Climate Wheat (Topic + Review)
21	Fuhrer, J.	2009	Ozone risk for crops and pastures in present and future climates.	Naturwissenschaften	Yield Climate Wheat (Topic + Review)
22	Garcia, G. et al.	2011	Variability of duration of pre-anthesis phases as a strategy for increasing wheat grain yield	Field Crops Research	Yield Variability Wheat (Title)
23	Gonzalez-Dugo, V.	2010	Water deficit and nitrogen nutrition of crops. A review	Agronomy for Sustainable Development	Water Wheat Yield (Topic + Review)
24	Hasanuzzaman, M. et al.	2013	Physiological, biochemical, and molecular mechanisms of heat stress tolerance in plants.	International Journal for Molecular Sciences	Heat Producti* Plant (Topic + Review)
25	Hatfield, J. et al.	2011	Climate Impacts on Agriculture: Implications for Crop Production	Agronomy Journal	cited by (Boote 2013)
26	Hossain, A. et al.	2011	Mechanisms of waterlogging tolerance in wheat: Morphological and metabolic adaptations under hypoxia or anoxia	Austr. J of Crop Science	Waterlogging Yield (Topic + Review)
27	Hay, R. et al.	1989	An introduction to the physiology of crop yield, 1st edition, by Hay and Walker	Longman Scientific & Technical	selected manually
28	Ishag, H. et al.	1996	Phasic development of spring wheat and stability of yield and its components in hot environments	Field Crops Research	Yield Stability Wheat (Title)
29	Jagadish, K. et al.	2014	Agronomic and Physiological Responses to High Temperature, Drought, and Elevated CO2 Interactions in Cereals	Advances in Agronomy	Yield Climate Maize (Topic + Review)
30	Juroszek, P. et al.	2013	Climate change and potential future risks through wheat diseases: a review	Eur J of Plant Pathology	Yield Climate Wheat (Topic + Review)
31	Lawlor, D. et al.	2009	Causes of decreased photosynthetic rate and metabolic capacity in water-deficient leaf cells: a critical evaluation of mechanisms and integration of processes	Annals of Botany	Drought Producti*
32	Leakey, A. et al.	2009	Elevated CO2 effects on plant carbon, nitrogen, and water relations: six important lessons from FACE	Journal of Experimental Botany	selected manually
33	Lobell, D. et al.	2012	Extreme heat effects on wheat senescence in India	Nature Climate Change	cited by (Boote 2013)
34	Lobell, D. et al.	2012	The influence of climate change on global crop productivity.	Plant Physiology	refers to (Hatfield 2011)
35	Lopes, M. et al.	2011	Enhancing drought tolerance in C4 crops.	Journal of Experimental Botany	Water Maize Yield (Topic + Review)
36	Luck, J. et al.	2011	Climate change and diseases of food crops	Plant Pathology	Yield Climate Wheat (Topic + Review)
37	Luo, Q.	2011	Temperature thresholds and crop production: a review	Climatic Change	Temperature Cereals Yield (Topic + Review)
38	Madhu, M. et al.	2013	Dynamics of Plant Root Growth under Increased Atmospheric Carbon Dioxide	Agronomy Journal	refers to (Hatfield 2011)
39	Miura, K. et al.	2013	Cold signaling and cold response in plants.	International Journal for Molecular Sciences	Cold Yield—Producti* Plant (Topic + Review)
40	Mohammed, A. et al.	2009	Impact of High Nighttime Temperature on Respiration, Membrane Stability, Antioxidant Capacity, and Yield of Rice Plants	Crop Science	Yield Stability Rice (Title)
41	Morison, J. et al.	1999	Interactions between increasing CO2 concentration and temperature on plant growth	Plant, Cell & Environment	Temperature Wheat Yield (Topic + Review)
42	Hay, R. et al.	2006	The Physiology of Crop Yield, 2nd edition, by Hay and Walker	Blackwell Publishing Limited	selected manually

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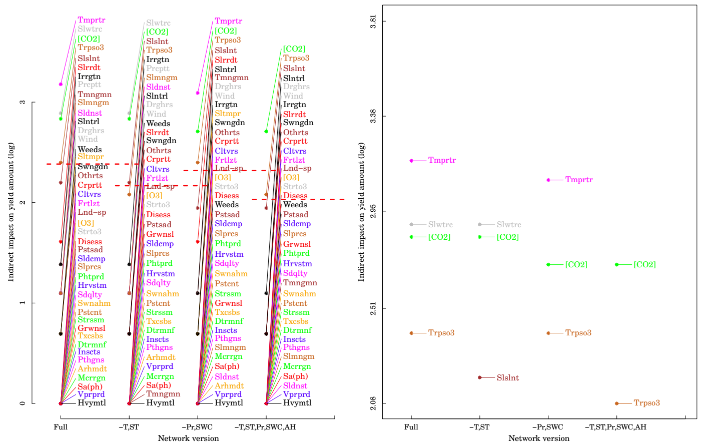
Table S2 – continued from previous page

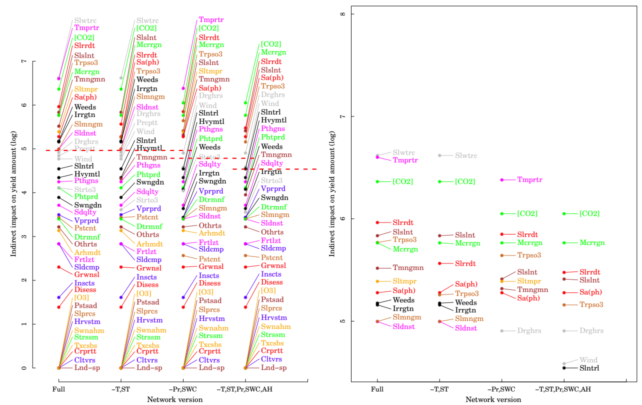
Nr	Author	Year	Title	Journal	Search term
43	Porter, J. et al.	1991	Plant Growth Interactions with nutrition and the environment, by Porter and Lawlor	Cambridge University Press	selected manually
44	Powell, N. et al.	2012	Yield stability for cereals in a changing climate	CSIRO Functional Plant Biology	Yield Stability Wheat (Topic + Review)
45	Hall, D. et al.	1993	Photosynthesis and Production in a changing environment, 1st edition, by Hall et al.	Chapman & Hall	selected manually
46	Larcher, W.	1995	Physiological Plant Ecology, 3rd edition, by Larcher	Springer	selected manually
47	Lambers, H. et al.	2008	Plant Physiological Ecology, 2nd edition, by Lambers et al.	Springer	selected manually
48	Reddy, A. et al.	2004	Drought-induced responses of photosynthesis and antioxidant metabolism in higher plants	Journal of Plant Physiology	Drought Yield (Topic + Review)
49	Roetter, R. et al.	1999	Climate change effects on plant growth, crop yield and livest	Climatic Change	Yield Climate Wheat (Topic + Review)
50	Sanchez, B. et al.	2014	Temperatures and the growth and development of maize and rice: a review	Global Change Biology	refers to (Barnabas 2008)
51	Schnyder, H. et al.	1993	The role of carbohydrate storage and redistribution in the source-sink relations of wheat and barley during grain filling - a review	New Phytologist	Yield Variability Grain filling (Topic + Review)
52	Siebenmorgen, T. et al.	2013	Impacts of preharvest factors during kernel development on rice quality and functionality.	Annual Review of Food Science and Technology	Yield Variability Grain filling (Topic + Review)
53	Suzuki, N. et al.	2014	Abiotic and biotic stress combinations	New Phytologist	Heat + Yield (Topic + Review)
54	Tambussi, E. et al.	2007	Water use efficiency in C3 cereals under Mediterranean conditions: a review of physiological aspects	Annals of Applied Biology	Yield Variability Growth (Topic + Review)
55	Thitisaksakul, M. et al.	2012	Effects of environmental factors on cereal starch biosynthesis and composition	Journal of Cereal Science	refers to (Barnabas 2008)
56	Tokatlidis, I.	2014	Addressing the yield by density interaction is a prerequisite to bridge the yield gap of rain-fed wheat	Annals of Applied Biology	Yield Climate Wheat (Topic + Review)
57	Wahid, A. et al.	2007	Heat tolerance in plants: An overview	Environmental and Experimental Botany	Heat + Yield (Topic + Review)
58	Yadav, S.	2010	Cold stress tolerance mechanisms in plants. A review	Agronomy for Sustainable Development	Cold Yield—Producti* Plant (Topic + Review)
59	Yang, J. et al.	2006	Grain filling of cereals under soil drying	New Phytologist	Water Rice Yield (Topic + Review)
60	Yu, Q. et al.	2014	Year patterns of climate impact on wheat yields	International Journal of Climatology	Yield Climate Wheat (Title)

Table S3: Keyword list applied for the literature search in the Web of Knowledge, together with the number of search results for topic, reviews with the topic, and title. A missing entry indicates that this search criterion was not applied (results were inspected at an earlier refinement stage, and no further filtering was performed).

Search term	Date	# Topic	# Topic and DT="Review"	Title
Yield Variability Wheat	15.05.2014	1844	41	71
Yield Stability Wheat	15.05.2014	1301	48	99
Yield Extremes Wheat	19.06.2014	280	14	
Yield Climate Wheat	21.07.2014	2018	118	95
Yield Variability Maize	05.08.2014	1155	32	47
Yield Stability Maize	05.08.2014	674	18	70
Yield Extremes Maize	05.08.2014	180	8	1
Yield Climate Maize	05.08.2014	1052	65	43
Yield Variability Rice	06.08.2014	594	25	25
Yield Stability Rice	06.08.2014	451	17	37
Yield Extremes Rice	06.08.2014	130	10	
Yield Climate Rice	06.08.2014	709	68	48
Yield Variability	21.07.2014	20582	669	531
Yield Extremes	21.07.2014	6458	281	36
Yield Variability Growth	13.01.2015	3428	110	22
Yield Variability Stomata	13.01.2015	28		
Yield Variability Stress	13.01.2015	1619	77	6
Yield Variability Transport	13.01.2015	1092	35	
Yield Variability Uptake	13.01.2015	593	15	
Yield Variability Photosynthesis	05.08.2014	426	23	1
Yield Variability Phenology	15.09.2014	203	5	2
Yield Variability Reproduction	15.09.2014	169	13	
Yield Variability Vernalization	15.09.2014	20	1	
Yield Variability Senescence	15.09.2014	93	4	
Yield Variability Evapotranspiration	15.09.2014	369	4	
Yield Variability Respiration	15.09.2014	196	7	
Yield Variability Cell Growth	15.09.2014	252	18	
Yield Variability Grain filling	15.09.2014	198	7	
Temperature Wheat Yield	13.01.2015	4285	110	
Temperature Rice Yield	13.01.2015	2430	67	
Temperature Maize Yield	13.01.2015	1687	43	
Temperature Cereals Yield	13.01.2015	646	46	
Water Wheat Yield	13.01.2015	8138	263	
Water Rice Yield	13.01.2015	3919	177	
Water Maize Yield	13.01.2015	3764	111	
Water Cereals Yield	13.01.2015	1229	95	
CO2 Wheat Yield	13.01.2015	1305	58	
CO2 Rice Yield	13.01.2015	640	45	
CO2 Maize Yield	13.01.2015	478	32	
CO2 Cereals Yield	13.01.2015	167	21	
Drought Yield	14.01.2015	8531	447	
(Water Logging OR Waterlogging) Yield	14.01.2015	1900	63	
Heat Yield	14.01.2015	40267	945	293
Cold AND (Yield OR Producti*)	19.01.2015	25467	1220	688
Cold AND (Yield OR Producti*) Plant	22.01.2015	3787	278	
Extreme AND (Yield OR Producti*)	22.01.2015	14543	932	188
Extreme AND (Yield OR Producti*) Plant	22.01.2015	1899	172	
Stress AND (Yield OR Producti*)	22.01.2015	136503	8964	4203
Stress AND (Yield OR Producti*) Plant	22.01.2015	22965	1787	139
Drought Producti*	22.01.2015	9857	693	
(Water Logging OR Waterlogging) Producti*	22.01.2015	2302	95	
Heat Producti*	22.01.2015	48413	2344	1961
Heat Producti* Plant	22.01.2015	6302	429	
CO2 Yield	26.01.2015	19150	580	
Carbon Dioxide Yield	26.01.2015	11735	463	
References to and from...				
[References to Barnabas 2008, PC&E]	13.01.2015	221		
[Citations in Barnabas 2008, PC&E]	13.01.2015	312		
[References to Boote 2013, PC&E]	13.01.2015	7		
[Citations in Boote 2013, PC&E]	13.01.2015	186		
[References to Farooq 2009, ASD]	22.01.2015	202		
[Citations in Farooq 2009, ASD]	22.01.2015	292		
[References to Hatfield 2011, AJ]	26.01.2015	78		
[Citations in Hatfield 2011, AJ]	26.01.2015	225		

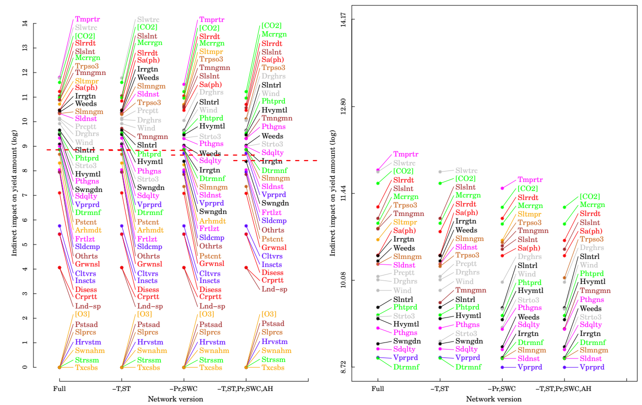


(a) Maximum path length = 2

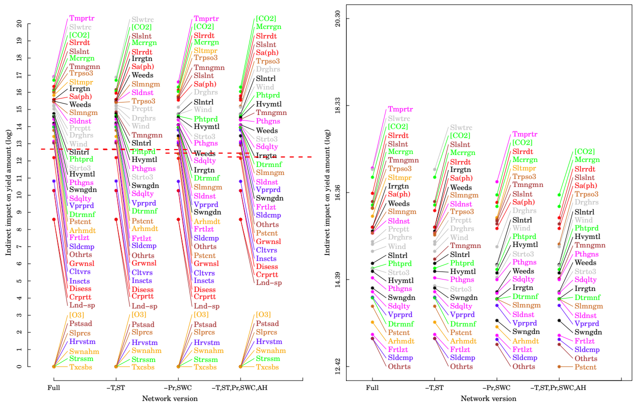


(b) Maximum path length = 4

Figure S4: [continued on next page]

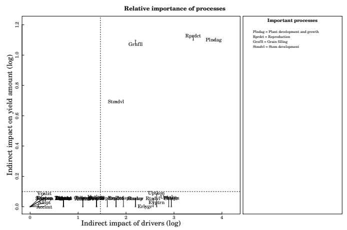


(c) Maximum path length = 7

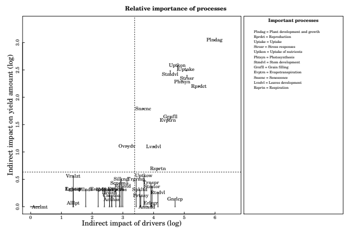


(d) Maximum path length = 10

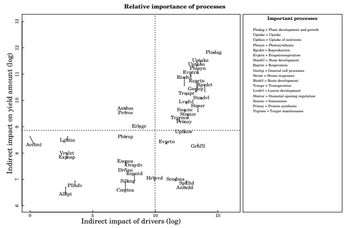
Figure S4: Analog to Figure 3.2 in the main paper the relative importance of environmental influences on yield amount. The left part contains all drivers in our network; the right part only contains the top 25% drivers (cutoff is indicated by the red lines in the left part; calculated after log-scaling). The different maximum path lengths allowed are a = 2, b = 4, c = 7, and d = 10. Abbreviation explanations can be found in Table S4; colors are assigned randomly to allow an easy distinction between entries.



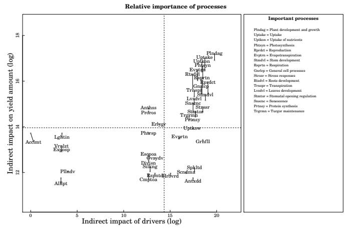
(a) Maximum path length = 1



(b) Maximum path length = 2

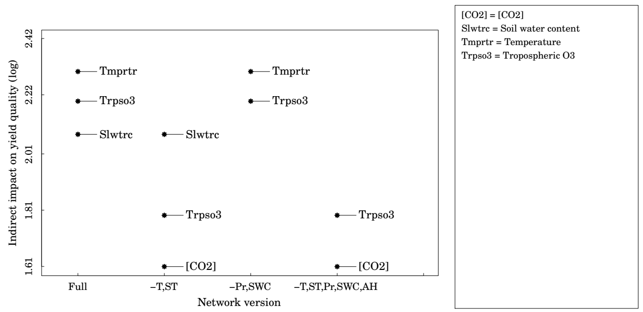


(c) Maximum path length = 7

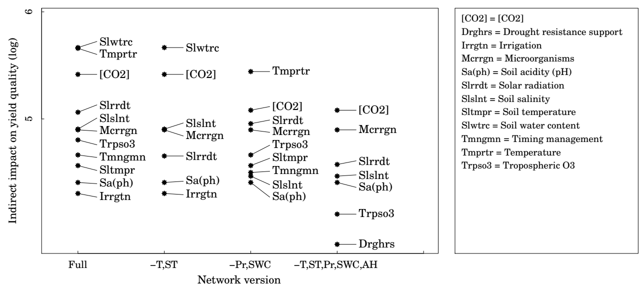


(d) Maximum path length = 10

Figure S5: Analog to Figure 3.3 in the main paper the relative importance of physiological plant processes is displayed. Each process is located according to the influence of environmental stimuli on it and its respective impact on yield amount. The different maximum path lengths allowed (a = 1, b = 2, c = 7, d = 10) are displayed at the top of each figure. Abbreviation explanations can be found in Table S4.

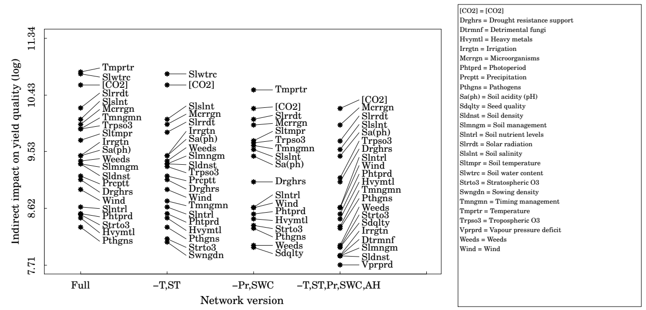


(a) Maximum path length = 2

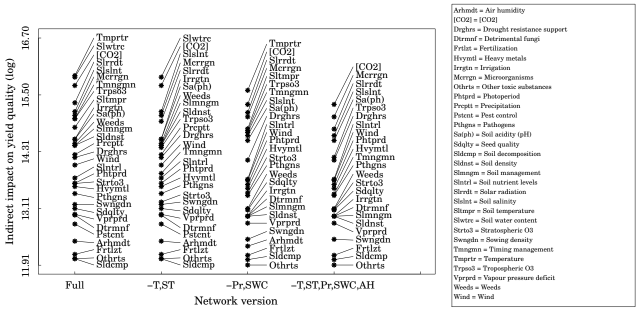


(b) Maximum path length = 4

Figure S6: [continued on next page]

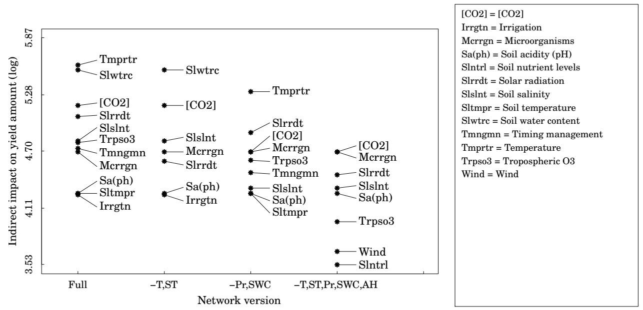


(c) Maximum path length = 7

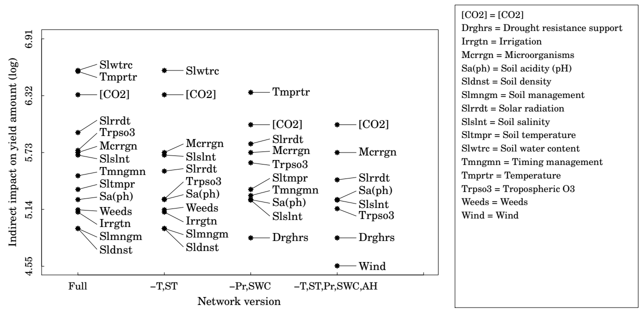


(d) Maximum path length = 10

Figure S6: Analog to Figure 3.2 in the main paper and Figure S4 in the supplement: the major environmental influences on yield **quality**. Only the top 25% drivers (calculated after log-scaling) drivers are displayed. The different maximum path lengths allowed are a = 2, b = 4, c = 7, and d = 10. Abbreviations in the right legends can be found in Table S4.

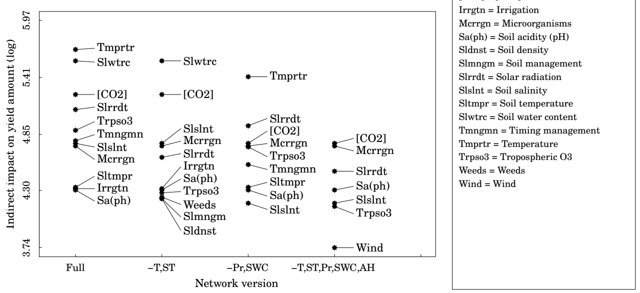


(a) Maize



(b) Wheat

Figure S7: [continued on next page]



(c) Rice

Figure S7: Analog to Figure 3.2 in the main paper the relative importance of environmental influences on yield amount is displayed, but split by crops: maize (a), wheat (b), rice (c). A maximum path length of 4 was allowed, and only the top 25% drivers are shown (calculated after log-scaling). Abbreviation explanations can be found in Table S4.

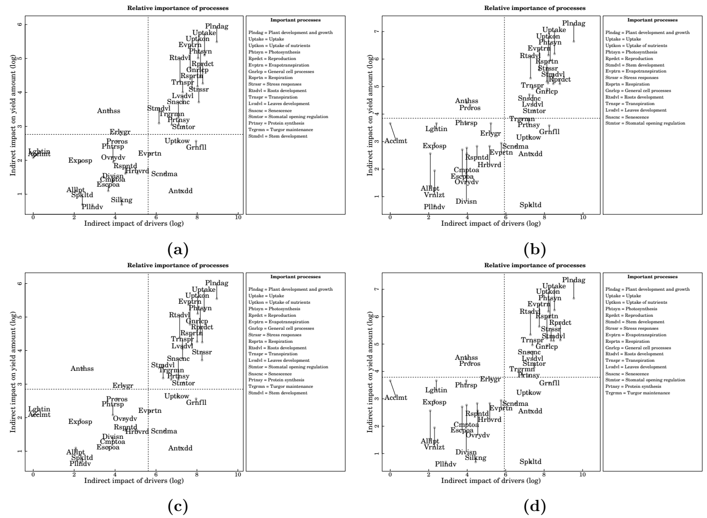


Figure S8: Analog to Figure 3.3 in the main paper: the relative importance of plant processes, split by crops (a = maize, b = wheat, c = rice, d = all crops). Importance is measured according to the influence that weather and other drivers exert on it (x-axis) and its respective influence on yield amounts (y-axis); see the methods section for details. The dashed horizontal and vertical lines represent the mean (of the log-ed values) of the x- and y-axis entries, respectively. The processes in the upper right corner are annotated in the legend on the right; these are sorted according to their Manhattan distance from the origin (i.e. the sum of x and y location). All other abbreviations are explained in Table S4.

Table S4: Abbreviations used in figures with their associated full process names (equal to network node names)

Abbreviation	Full process/node name	Abbreviation	Full process/node name
[CO2]	[CO2]	Prtncn	Protein content
[O3]	[O3]	Prtnsy	Protein synthesis
Acclmt	Acclimation	Pstcnt	Pest control
Alllpt	Allelopathy	Pstsad	Pests and diseases
Anthss	Anthesis	Pthgns	Pathogens
Antxdd	Antioxidant defense	Rprdct	Reproduction
Arhmdt	Air humidity	Rspntd	Responses to diseases
Cltvrs	Cultivar selection	Rsprtn	Respiration
Cmptoa	Compatible osmolytes accumulation	Rtsdvl	Roots development
Crprtt	Crop rotation	Sa(pH)	Soil acidity (pH)
Disess	Diseases	Scndma	Secondary metabolites accumulation
Divisn	Division	Sdqlty	Seed quality
Drghrs	Drought resistance support	Silkng	Silking
Dtrmnf	Detrimental fungi	Sldcmp	Soil decomposition
Erlygr	Early growth	Sldnst	Soil density
Escpoa	Escape or avoidance	Slmngm	Soil management
Evprtn	Evaporation	Slntrl	Soil nutrient levels
Evptrn	Evapotranspiration	Slprcs	Soil processes
Exposp	Expression of stress proteins	Slrrdt	Solar radiation
Frtlzt	Fertilization	Slslnt	Soil salinity
Gnrlcp	General cell processes	Sltmpr	Soil temperature
Grnfll	Grain filling	Slwtrc	Soil water content
Grnfrm	Grain form	Snscnc	Senescence
Grnnmb	Grain number	Spkltd	Spikelet development
Grnwos	Grain weight or size	Stmdvl	Stem development
Grwnsl	Growing season length	Stmtor	Stomatal opening regulation
Hrbvrd	Herbivory defenses	Strssm	Stress mitigation
HrviHI	Harvest index HI	Strssr	Stress responses
Hrvstm	Harvesting method	StrtO3	Stratospheric O3
Hvymtl	Heavy metals	Swnahm	Sowing and harvesting management
Inscts	Insects	Swngdn	Sowing density
Irrgtn	Irrigation	Tmngmn	Timing management
Lghtin	Light interception	Tmprtr	Temperature
Lnd-sp	Land-use patterns	Trgrmn	Turgor maintenance
Lvsdvl	Leaves development	Trnspr	Transpiration
Mcrntr	Micronutrients	TrpsO3	Tropospheric O3
Mcrrgn	Microorganisms	Ttlamn	Total amount
Othrts	Other toxic substances	Txcsbs	Toxic substances
Ovrydv	Ovary development	Uptake	Uptake
Phtprd	Photoperiod	Uptkon	Uptake of nutrients
Phtrsp	Photorespiration	Uptkow	Uptake of water
Phtsyn	Photosynthesis	Vprprd	Vapor pressure deficit
Pllndv	Pollen development	Vrnlzt	Vernalization
Plndag	Plant development and growth	Weeds	Weeds
Prcptt	Precipitation	Wind	Wind
Prcssa	Processing attributes	Yldamn	Yield amount
ProROS	Production of ROS	Yldqlt	Yield quality

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3 Global historical soybean and wheat yield losses from ozone

This chapter is based on a manuscript that is currently (June 28, 2017) under review at Global Change Biology (at John Wiley and Sons). The authors are Bernhard Schauberger, Susanne Rolinski, Sibyll Schaphoff and Christoph Müller; all at the Potsdam Institute for Climate Impact Research (PIK). The submission title is "Global historical soybean and wheat yield loss estimates from ozone pollution considering water and temperature as modifying effects".

3.1 Article

Abstract

Ozone pollution can severely diminish crop yields. Its damaging effects depend, apart from ozone concentration, on crop, cultivar, water status, temperature and CO_2 concentration. Previous studies estimating global yield loss from ozone pollution did not consider all of these cofactors and climate change impact studies on crop yields typically ignore ozone pollution. Here we introduce an ozone damage module for the widely used process-based crop model LPJmL. The implementation describes the ozone uptake through stomata, internal detoxification and short- and long-term effects on productivity and phenology, dynamically accounting for all listed cofactors. Using this extended model we estimate historical global yield losses from ozone pollution for wheat and soybeans. We divide wheat into Western and Asian types to account for different sensitivities towards ozone. We apply daily ozone concentrations obtained from four chemistry-transport models provided by the ACCMIP project.

Our implementation of ozone damage follows expected dynamics, for example an amplification of damages under irrigation. The model is able to reproduce results from chamber and field studies. Historical losses between 2001 and 2005 vary between countries and we estimate these to range between 0 and 12% of ozone-free yields for soybeans, between 1 and 22% for Western wheat and between 10 and 53% for Asian wheat.

Our study highlights the threat of ozone pollution for crop production. Uncertainties of our study include the extrapolation from rather few point observations to the globe, possible biases in ozone data, omission of sub-daily fluctuations in ozone concentration or stomatal conductance and the averaging of different cultivars across regions. We suggest performing further field-scale experimental studies of ozone effects on crops, as these are currently rare but would be particularly helpful to evaluate models and to estimate large-scale effects of ozone.

Introduction

High levels of surface ozone (O_3) can lower crop yields substantially (Burney & Ramanathan, 2014, Fuhrer, 2009, Ghude *et al.*, 2014, Long *et al.*, 2005, McGrath *et al.*, 2015, Mills *et al.*, 2015). Up to date, pollutants including ozone may even have contributed more to yield changes than climate change (Shindell, 2016). Ozone is a powerful oxidant and the mechanisms how it affects plants are well understood (Ainsworth *et al.*, 2012, Wilkinson & Davies, 2010, Wilkinson *et al.*, 2012). The gas enters plant leaves via the stomata and swiftly reacts with apoplast components to form reactive oxygen species (ROS). These react further with membranes and cell components and cause damages to enzymes, including photosynthesis proteins. This leads to lower rates of carbon (C) assimilation. To prevent damage plants tend to lower stomatal conductance in the presence of O_3, causing reduced influx of CO_2 and thus also lower photosynthesis rates. Senescence is advanced with higher O_3 due to accumulating damages, causing a precocious loss of green leaf area. A share of assimilated carbon is respired for repairing ozone-induced damages and to build up anti-oxidant defenses like ascorbate. All these effects lead to a lower net assimilation of C on short and long term, eventually resulting in lower yield levels. Additionally, ovary sterility or kernel abortion could ensue from ozone damage, leaving less sink capacity for yield formation. Weather conditions favorable for O_3 formation (dry, sunny and warm) may cause stress for plants, while their capacity to cope with stress is diminished due to O_3 (Wilkinson *et al.*, 2012). Wheat and soybean are deemed particularly sensitive to O_3 (Feng *et al.*, 2008, McGrath *et al.*, 2015, Wilkinson *et al.*, 2012). Ozone is also a greenhouse gas accelerating climate change and thus affecting yields indirectly (Fishman *et al.*, 1979, Sitch *et al.*, 2007).

Ozone formation in the atmosphere is complex (Rai & Agrawal, 2012), largely determined by three limiting factors: solar radiation, temperature and amount of precursors (methane, carbon monoxide and NO_x compounds). These factors can vary independently (Fuhrer, 2009, McGrath *et al.*, 2015), leading to substantial variance in O_3 levels over space and time (Lin *et al.*, 2015, Stevenson *et al.*, 2006). Ozone trends diverge between regions. While in industrialized countries concentrations increased previously but have stabilized or declined due to stricter enforcement of thresholds, O_3 trends are upwards in transition economies like India and China (Rao *et al.*, 2016, The Royal Society, 2008). Quantifying the global impact of O_3 on crop yields is thus a pertinent issue.

There are numerous chamber and field studies quantifying the effect of increased O_3 on yields, reviewed, for example, by Broberg *et al.* (2015), Feng *et al.* (2008), Long *et al.* (2005), Morgan *et al.* (2003) or Rai and Agrawal (2012). Modeling studies based on experiments can be divided into two categories: exposure-response functions (ERF) for empirical correlations between yield and ozone exposure, and process-based models simulating physiological effects of O_3 on different plant processes. ERF's are readily computed for large geographical areas and produce reliable results under similar conditions as they were trained on (Musselman *et al.*, 2006, Pleijel *et al.*, 2007). Examples of ERF applications comprise Avnery *et al.* (2011) or Van Dingenen *et al.* (2009) where the authors calculate ozone damages for soybean, wheat and other crops in 2000, estimating losses between 4 and 16% depending on crop and region. Chuwah *et al.* (2015) study effects on eleven crops between 2005 and 2050 and derive that at least 2.5% of additional cropland area would be required to compensate for O_3-induced production losses. Avnery *et al.* (2013) research two pathways to reduce crop damage: climate change mitigation or crop adaptation. Burney and Ramanathan (2014) apply damage functions to estimate wheat and rice loss in India, correlating yield with O_3 precursors rather than O_3 concentrations directly, due to a lack of data. Tai *et al.* (2014) study interactive effects between O_3 and temperature changes in 2000 and 2050 for four crops and assess the impact on food security. But these ERF-based assessments are agnostic about the underlying mechanisms how O_3 reduces yields. Additionally, interactions between O_3 and other environmental factors like CO_2 or water stress are usually not considered. Approaches that account for actual fluxes to the leaves, rather than outside concentrations, are thus necessary to complement experimental studies (Ainsworth *et al.*, 2012, Franz *et al.*, 2017). These could support adaptation or plant breeding for more O_3-resistant cultivars.

Few process-based crop models including ozone stress have been designed. A hybrid between process-based and empirical model is the DO$_3$SE model by Emberson *et al.* (2000). Stomatal conductance is described in dependence of limiting factors including water stress, light, temperature and ozone. The resulting stomatal ozone flux can be distinct from concentrations. Another semi-empirical damage function is derived by Reilly *et al.* (2007) who calculate economic effects of interacting CO_2, O_3 and climate change on crop yields. But they only consider a generic C_3 crop on monthly time step. Fuhrer (2009) developed a model for O_3 damage with explicit stomatal conductance and detoxification, but remained on a conceptual basis. Sitch *et al.* (2007) assessed indirect effects of O_3 on climate change, but considered only generic vegetation and crops. Finally, Ewert and Porter (2000) provide a detailed study of CO_2 and O_3 interactive effects on wheat yields. They consider short-term (reduced photosynthesis) and long-term (advanced senescence) damages of O_3, but omit water stress effects, possible costs of cell repair measures and do not provide global assessments.

In this study, we extend the global vegetation and crop model LPJmL (Bondeau *et al.*, 2007) towards ozone effects on crops. We model the effect of historical O_3 concentrations on global wheat and soybean yields. We explicitly consider interaction effects of O_3 with temperature, water stress, phenology and CO_2. We separately analyze Western (i.e. European and North American) and Asian wheat varieties to account for differences in their ozone responses (Emberson *et al.*, 2009, Feng *et al.*, 2012). This is, to our knowledge, the first study analyzing ozone-induced yield losses at the global scale with consideration of modulating co-factors.

Materials and methods

<u>Crop model and crops</u>

LPJmL is a widely used, process-based dynamic vegetation and crop model (Bondeau *et al.*, 2007, Sitch *et al.*, 2003, Waha *et al.*, 2012). LPJmL simulates carbon (C) cycling and vegetation dynamics with explicit representation of physiological processes. These include photosynthesis, autotrophic respiration, water transpiration, evaporation, interception and runoff in natural and agricultural systems. The model is driven by daily weather (temperature, precipitation, incoming shortwave radiation and net downward longwave radiation), atmospheric CO_2 concentrations and soil texture. Agriculture is described by managed grasslands and twelve crop functional types that differ in bio-climatic limits and eco-physiological parameters. Photosynthesis and acquisition of carbon is based on BIOME3 (Haxeltine & Prentice, 1996a). Stomatal conductance is optimized to maximize carbon assimilation while simultaneously minimizing water loss. Net assimilated C is allocated to four crop compartments: root, stem including mobile reserves, leaves and storage organs. Yield is represented by the amount of C in storage organs. In this study, LPJmL operates on 0.5° grid cells (approx. 50 km at the equator) with individual land-use fractions and irrigation shares. Sowing and harvesting dates for crops are calculated internally considering climatic histories (Waha *et al.*, 2012). LPJmL uses a potential productivity scaling factor accounting for management differences between countries: LAI_{max}, the maximum Leaf Area Index the plant can achieve under optimum conditions, ranging between 1 and 7 (Fader *et al.*, 2010). This factor is calibrated per country and crop such that temporally averaged national yield levels simulated by LPJmL and reported by FAO (FAO, 2016) agree (SI Figure S1). For assessing its influence we perform loss calculations also with globally constant (high) management intensity.

We consider two staple crops, wheat and soybean, which together cover 22% of the global harvested area (Portmann *et al.*, 2010). Since Asian and European/North American ("Western") wheat varieties are known to react differently to ozone (Emberson *et al.*, 2009, Feng *et al.*, 2012) we separately consider these two types. For soybean this distinction is not made since differences are currently unclear (Emberson *et al.*, 2009). A choice between spring and winter wheat is computed internally by LPJmL, depending on climatic suitability with a preference for winter wheat.

<u>Modeling ozone effects</u>

The complex interaction of ozone with crops is simplified to three steps in our model (Figure 1, Table 1). First, O_3 outside the leaf ($O_{3,out}$) is taken up via the stomata, leading to an inner concentration $O_{3,in}$. Stomatal conductance for O_3 is derived from the conductance for water vapor by dividing by 1.6 (difference in diffusion coefficients of CO_2 and water vapor, (Haxeltine & Prentice, 1996a)) and by 1.075 to account for differences between CO_2 and O_3 (Ewert & Porter, 2000). The concentration of O_3 in cells is virtually zero (Ewert & Porter, 2000, Plöchl *et al.*, 2000), as other oxidizing agents (reactive oxygen species, ROS) are quickly formed. We do not resolve these reactions for the sake of model simplicity. Second, $O_{3,in}$ is lowered by a detoxification process in cells and cell walls (Castagna & Ranieri, 2009, Plöchl *et al.*, 2000) that reduces $O_{3,in}$ to a harmful concentration $O_{3,harm}$. This process is split into two parts: an amount of $O_{3,in}$ is scavenged at no additional cost to the plant (owed to a basal rate of antioxidants production), while the remaining fraction requires energy to be detoxified and thus increases respiration (Dizengremel *et al.*, 2008, Ewert & Porter, 2000, Franz *et al.*, 2017, Fuhrer *et al.*, 1997). Franz *et al.* (2017) state that about half of external O_3 is taken up and detoxified via non-stomatal pathways (Kollist *et al.*, 2000, Tuzet *et al.*, 2011, Yin & Struik, 2009) and that this O_3 destruction pathway is important when assessing risks for plants. We do not directly account for these effects, but model them as subsumed with the general detoxification. We do also not explicitly account for damage recovery, which is particularly relevant for younger leaves (Ewert & Porter, 2000), but subsume this effect in the detoxification process. We assume this as valid surrogate since damage repair requires energy as well. Since LPJmL employs a big-leaf approach, the distinction between younger and older leaves is currently not possible. Third, the inner harmful concentration $O_{3,harm}$ leads to damages: gross photosynthesis is reduced (short-term damage) and senescence is advanced (long-term), thereby shortening the time to acquire biomass and yield. Senescence is advanced for both wheat and soybeans, but only for soybeans also the maturity time point is advanced. There is no literature reference for neither advancing nor constant maturity of soybeans under elevated O_3, but we assume this for two reasons: a delayed development under elevated CO_2 (Castro *et al.*, 2009), having in mind that O_3 is an antagonist of CO_2, and derivations of earlier maturity times based on decreasing chlorophyll contents in plants in one experiment (Betzelberger *et al.*, 2010). For wheat, maturity is not advanced due to contrasting evidences from the literature (Feng *et al.*, 2008, Feng *et al.*, 2011, Zhu *et al.*, 2011).

These three steps are added to the existing photosynthesis model (Table 1). Potential damages of O_3 to the stomata (Hoshika *et al.*, 2015, Mills *et al.*, 2009), which would affect O_3 uptake in the long term, are not considered due to data scarcity for crops. Similarly, the direct sensing of O_3 by stomata, with subsequent closure independent of photosynthesis (Lombardozzi *et al.*, 2012), is not simulated due to data scarcity for crops. CO_2 fertilization of crops is considered in LPJmL (Bondeau *et al.*, 2007, Haxeltine & Prentice, 1996a, Haxeltine & Prentice, 1996b) and affects the response of crops to O_3 via its effect on stomatal conductance: higher concentrations of CO_2 result in lower stomatal conductance, which in turn allows less O_3 to enter the leaves. The two molecules therefore act as antagonists: the more there is of one, the less the other will diffuse into leaves since both can lower stomatal conductance.

After calculating an optimized stomatal conductance that accounts for temperature, water, ozone and CO_2 concentration, the actual C assimilation, C allocation and daily evapotranspiration are calculated. All other steps in LPJmL are as described in Bondeau *et al.* (2007).

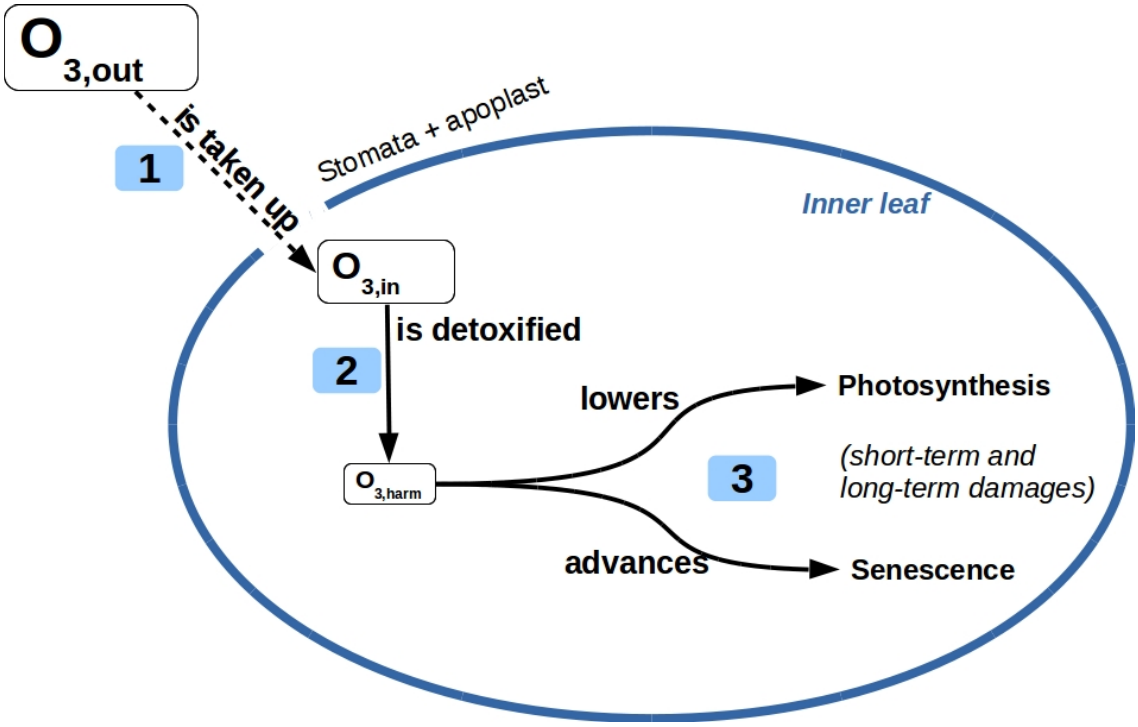


Figure 1: *Reaction scheme of ozone as modeled in LPJmL. The size of O_3 boxes reflects their relative concentrations. Numbers refer to the three steps as described in text and Table 1. Abbreviations are $O_{3,out}$: outer ozone concentration (in ppbv), $O_{3,in}$: inner ozone/oxidative agent concentration (blurring over the fact that O_3 concentration inside cells is virtually zero), $O_{3,harm}$: harmful inner concentration.*

Table 1: *Equation adaptations in LPJmL to account for ozone stress. Adaptations to the default LPJmL equations are underlined. Units of values are omitted for clarity.*

Step	**Process**	**Affected variable**	**Equations**	**Comment**
1	Uptake	Stomatal conductance	$\lambda \sim \underline{\min(}gc(water; CO_2)\underline{, gc(O_3; CO_2))}$	Lambda (λ) is the relation between inner and outer [CO_2] with a maximum of 0.8. Water-limited and O_3-limited lambda are separately optimized, then the minimum of

Step	Process	Affected variable	Equations	Comment
				these two is taken to represent stomatal conductance[1].
		Inner $[O_3]$	$\underline{O_{3,in} = O_{3,out} * \lambda / \lambda_{max} * gc_{max}}$	Relation between inner and outer O_3 depends on stomatal conductance, represented by λ over λ_{max} (0.8) times the maximum conductance under no stress.
2	Detoxification	Basic scavenging	$\underline{O_{3,in} = max(0, O_{3,in} - bs_{PFT})}$	A certain amount of O_3 is not harmful for the plant and is scavenged without additional energy costs.
		Respiration	$rd = b_{C3} * V_{max} \underline{* (1 + r_{PFT} * O_{3,in})}$	The remaining O_3 increases cell respiration, for repairing and scavenging.
		Harmful $[O_3]$	$\underline{O_{3,harm} = O_{3,in} * (1 - d_{PFT})}$ $\underline{O_{3,harm.cum} = O_{3,harm.cum} + O_{3,harm}}$	O_3 is reduced by a percentage to the remaining harmful concentration. The cumulative harmful concentration $O_{3,harm.cum}$ is calculated (set to 0 at sowing).
3	Damage	Reduction of jc	$jc = c_{C3} * V_{max} \underline{* max(0, 1 - j_{PFT} * O_{3,harm})}$	Rubisco-limited photosynthesis *jc* is reduced by O_3. See comments on V_{max} in the discussion.
		Senescence onset	Senescence starts when $HU_{sum} / HU_{max} > fracsen$ **Wheat:** $fracsen = 0.7 * \underline{max(0, 1 - s_{PFT} * O_{3,harm.cum})}$ **Soybeans:** $HU_{sum} = HU_{sum} + hu * vrf * prf * \underline{(1 + s_{PFT} * O_{3,harm.cum})}$	Advancing of senescence is realized by lowering the PHU threshold necessary to reach senescence (wheat) or by enhancing the gain of PHUs (soybeans). The value of 0.7 (equal for wheat and soybeans) is the fraction of maximum heat units (HU_{max}) necessary for senescence onset. HU_{sum} gain is modified by vernalization (vrf) and photoperiodic (prf) factors.

[1] This is physiologically inaccurate since the interaction between water stress and O_3 would best be represented by a hyperplane. But the separate optimization saves computation time and avoids the data gap on the interactive response.

Parameter calibration

The ozone module requires five crop-specific parameters: bs_{PFT} (in mmol/m^2/day) describing the basal scavenging without energy cost, d_{PFT} (between 0 and 1, unitless) describing the fraction of $O_{3,in}$ that is detoxified at the cost of higher respiration, r_{PFT} (mmol^{-1}m^2 *day) describing the respiration increase for this detoxification, j_{PFT} (mmol^{-1}m^2 *day) describing the Rubisco (i.e. ribulose 1,5-bisphosphate carboxylase/oxygenase)-limited photosynthesis penalty due to ozone and s_{PFT} (mmol^{-1}m^2) describing the advance in senescence (and phenology for soybeans). No literature values were available for these parameters, thus they were subjected to a calibration aiming to reproduce experimental studies. After a first round of calibration, where all five parameters were free, it became obvious that there are pairwise inverse correlations that require some parameters to be fixed. We decided to fix bs_{PFT} and r_{PFT} , to which the model is either not very sensitive (r_{PFT}, Figure 4) or there is an orientation value (bs_{PFT}). We fixed bs_{PFT} at 0.16 mmol m^{-2} day^{-1}, corresponding to a threshold of a non-damaging O_3 concentration of 40 ppbv (as in the AOT40 exposure metric often used as non-damaging in ERF studies, e.g. Avnery *et al.* (2011) or Fuhrer *et al.* (1997)) at a maximum stomatal conductance of 6 mm sec^{-1} (equal to 0.162 mol m^{-2} sec^{-1} of conductance to O_3 at 25°C and 1000 hPa pressure) for 8 hours. The fixed value of r_{PFT} was determined by a linear regression using experiments (all where respiration was provided; SI Table S1). Other crop-specific parameters like base temperatures or allocation constraints were not calibrated since these are based on literature values (Bondeau *et al.*, 2007). No scaling from leaf to plant was used, i.e. the whole plant was treated as one big leaf.

Calibration was performed by traversing a full three-dimensional cube with 20 values for each of the three parameters to be calibrated (d_{PFT}, j_{PFT}, s_{PFT}), resulting in a total of 20^3 = 8,000 model runs. Values were iterated, ranging from 0.05 to 5.0 times of the starting value (j_{PFT}, s_{PFT}) derived from linear regressions using experimental evidence, or between 0 and 100% (d_{PFT}). The weighted average root mean square error (RMSE) was used as target function, calculated for all pairs of observed and simulated variables. The weights for calibration variables were: 2 for the O_3 flux to leaves, 2 for stomatal conductance, 1 for A_{sat} as percentage of control, 1 for relative yield loss and 0.1 for respiration. Stomatal conductance and ozone uptake were weighed highest since these are the decisive processes that allow an upscaling from experimental to global level. Reduction in A_{sat} and relative yield loss are of second importance since these are used as a mixture of result (from ozone uptake) and independent observation. Respiration was weighed least since experimental values were judged uncertain. Resulting RMSE values were often similar (difference only in the third or fourth decimal place) such that of the 100 simulations with the lowest RMSE values the parameter set with the lowest penalty factors was chosen. This is justified by lower observed damages in reality than in experiments (Morgan *et al.*, 2003). The LAI_{max} management parameter was adapted for each experiment before calibration such that the control yield level was correctly simulated.

The Web of Science® was searched in spring 2016 for experimental studies that described ozone effects on wheat or soybean and reported one or more physiological observations useful for calibration (yield loss, O_3 uptake, light-saturated photosynthesis, stomatal conductance, respiration and/or growing season length). Six different studies containing 16 experiments were considered for Western wheat, seven studies with 12 experiments for Asian wheat and four studies with 11 experiments for soybeans (SI Table S1). The experimental conditions described in these studies, including in particular O_3 and CO_2 concentrations, water provision and temperature, were provided as input for LPJmL. Output variables for comparison were extracted from the manuscripts, involving the use of digitizing software (*engauge*[2]).

An out-of-sample calibration was performed to evaluate the reliability of the calibration process. Each experiment was omitted from calibration in turn and the best parameters identified for the reduced experiment set. Simulation results for the omitted experiment were then calculated with these out-of-sample calibrated parameters.

Ozone data

The ideal historical ozone data set for this exercise would contain daily surface O_3 concentrations, as mass or volume mixing ratio, over several years on the whole globe on a 0.5° spatial resolution. But such a data set does not exist. Therefore we use an ensemble of daily global surface ozone concentrations, derived from chemical transport models participating in the ACCMIP model inter-comparison (Lamarque *et al.*, 2013). Four models are included in the ensemble: GEOSCCM, GFDL-AM3, MIROC-CHEM and UM-CAM provided hourly data around the year 2000. Hourly data were aggregated to daily data by extracting, separately for each model, the daily mean and maximum concentration between 8 am and 4 pm and constructing a weighted average of these two values: a 'low' average

[2] http://markummitchell.github.io/engauge-digitizer/; accessed on March 08, 2017

assigns double weight to the mean, while a 'high' average assigns double weight to the maximum concentration. The daily aggregates were then downscaled from model resolution to 0.5° spatial resolution with a double-conservative remapping that conserves fluxes and spatial gradients. From these downscaled daily values a 'high' and a 'low' ensemble were created by taking the median of the four models in the respective low or high setting. The usage of model ensembles is motivated by a better agreement of ensemble than single-model values with observed data (Fiore *et al.*, 2009). The data flow for ozone input preparation is shown in SI Figure S2. A comparison of both 'low' and 'high' ensemble to observed values can be found in SI Figure S3.

Climate and land-use data

Temperature, precipitation, shortwave and longwave solar radiation are taken from the WFDEI data set (Weedon *et al.*, 2014). These data have often been used by climate change impact models (Warszawski *et al.*, 2014), and in particular in the Agricultural Model Intercomparison and Improvement Project's (AgMIP) global gridded crop model inter-comparison, GGCMI (Elliott *et al.*, 2015).

Crop-specific land-use and irrigation fractions are extracted from the MIRCA2000 data set on 0.5° spatial resolution, representative of the global crop distribution around the year 2000 (Portmann *et al.*, 2010). These fractions are held fixed to limit potential co-variation of O_3 damages and land-use shifts. Growing seasons are computed internally by LPJmL (Waha *et al.*, 2012).

Model evaluation

Four levels of model evaluation were applied. First, the model was tested against experimental observations. These studies were also used to calibrate model parameters, once with the full data set and once as an out-of-sample calibration. Second, sensitivity runs were performed where either input variables or model parameters were varied. These runs were not compared to observations, but gave insights whether the inner mechanics of the model were reasonable. Third, simulated national yield losses were compared to previous studies by McGrath *et al.* (2015), Ghude *et al.* (2014) and Burney and Ramanathan (2014). Fourth, the global historical loss estimates produced by LPJmL were compared to previous estimates using Exposure Response Functions (ERFs).

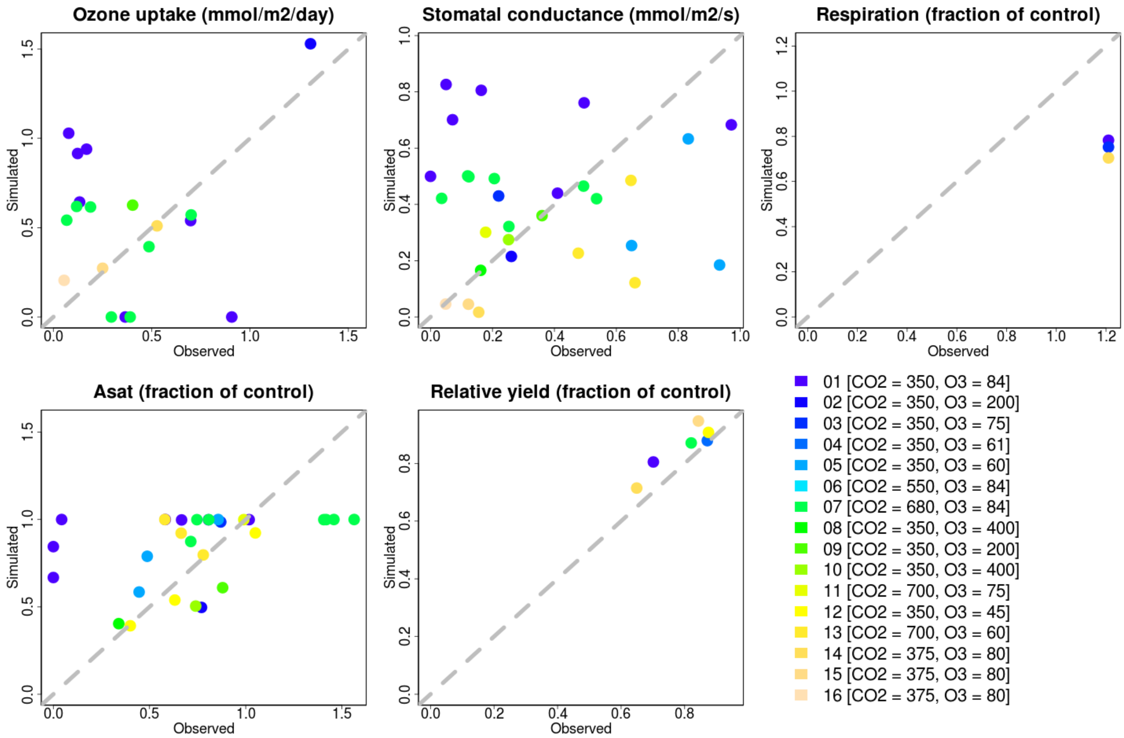
Results

Parameter calibration

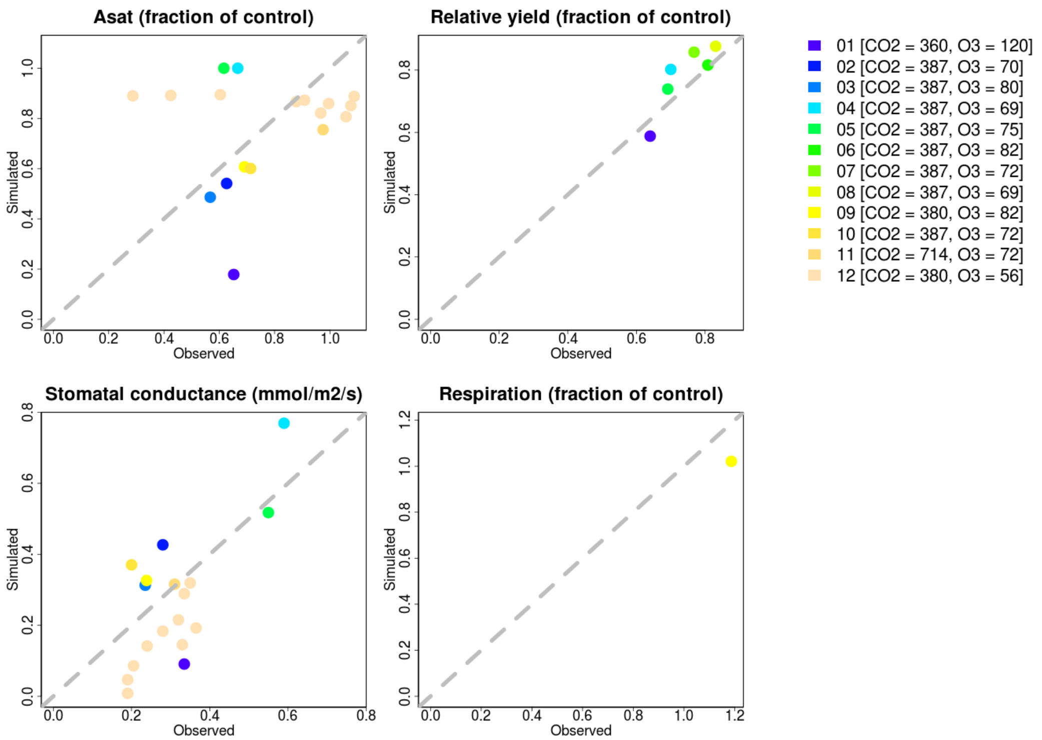
The calibration procedure leads to crop-specific parameter sets (Table 2). Asian and Western wheat parameters differ in the detoxified percentage, the photosynthesis penalty and the respiration increase; all of them show larger effects of O_3 on Asian wheat. Calibration plots for each crop (Figure 2) show the agreement between experimentally observed and simulated values for ozone uptake, light-saturated (i.e. Rubisco-limited) photosynthesis A_{sat}, stomatal conductance for water and relative yield loss. For each of the variables different counts of observations are available. Ideally all points would lie on the 1:1 line shown for comparison. Out-of-sample calibration shows that the results are very robust towards omission of single experiments (SI Figure S4). Stomatal conductance and ensuing ozone uptake show substantial variation around the 1:1 line, but with no systematic bias, and generally match with observations in dynamics and magnitude (except stomatal conductance for soybeans in two experiments). Note that ozone uptake is not measured for any experiment with Asian wheat. Relative yield loss is estimated rather conservatively for all three crops – there is, with one exception, no simulation below the 1:1 line.

***Table 2**: Calibrated values for the five O_3 parameters*

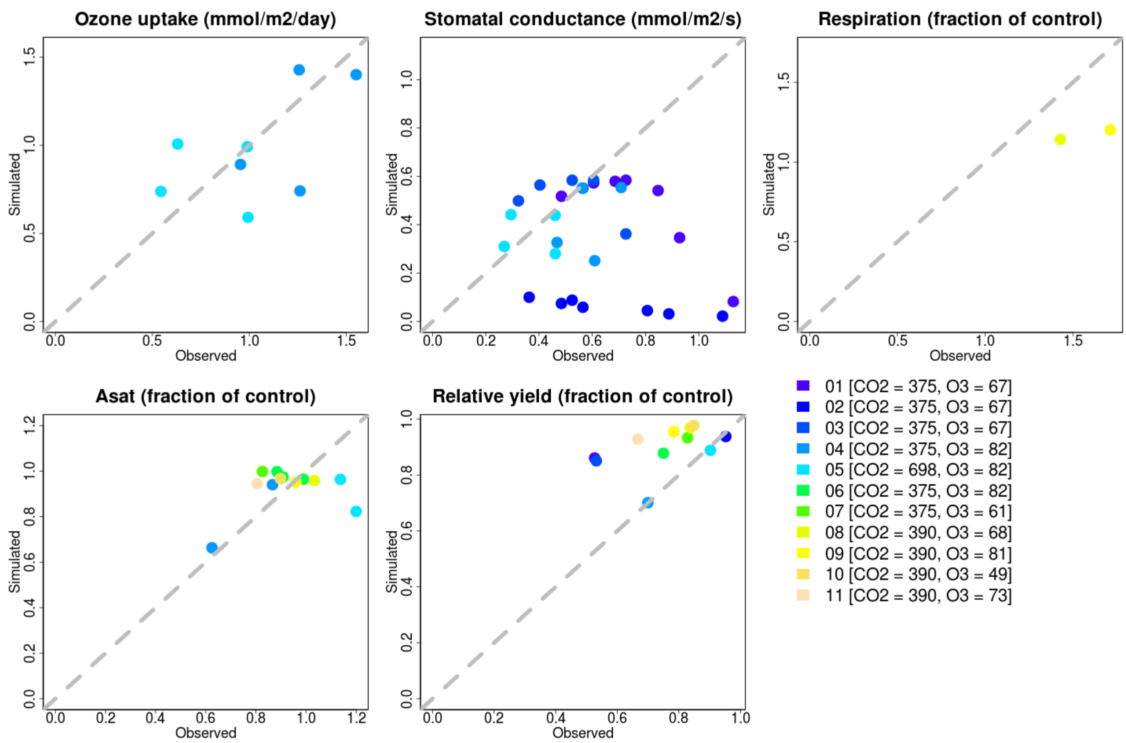
Parameter	**Western wheat**	**Asian wheat**	**Soybeans**	**Comment**
bs_{PFT}	0.1600	0.1600	0.1600	Fixed value
d_{PFT}	0.7916	0.5832	0.7916	
r_{PFT}	0.1000	0.1729	0.9470	Fixed value
j_{PFT}	0.0100	3.0000	0.2590	
s_{PFT}	0.0739	0.0792	0.0250	



(a) Western wheat



(b) Asian wheat



(c) Soybeans

***Figure 2**: Calibration results for all three crops: **(a)** Western wheat, **(b)** Asian wheat, **(c)** soybeans. Subpanels show experimentally observed values on the x-axis and simulated values on the y-axis. Different colors denote different experiments; detailed descriptions are listed in SI Table S1. There can be several measurements of one variable within one experiment.*

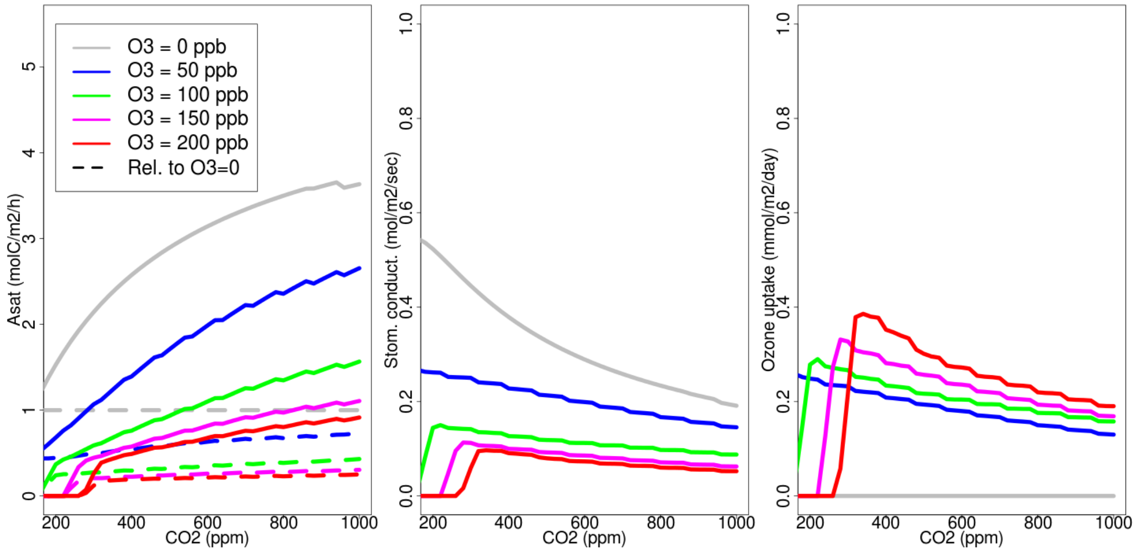
Sensitivity towards weather or parameter variation

Sensitivity of the model towards input variation is displayed in Figure 3, similar to the tests conducted by Ewert and Porter (2000). Asian wheat is shown here; the other crops convey similar dynamics (SI Figure S5). Since phenological development, in particular the LAI, influences photosynthetic performance, analogous plots without senescence advancing can be found in SI Figure S6 – with different dynamics, but similar patterns (except ozone uptake monotonically increasing with exposure time).

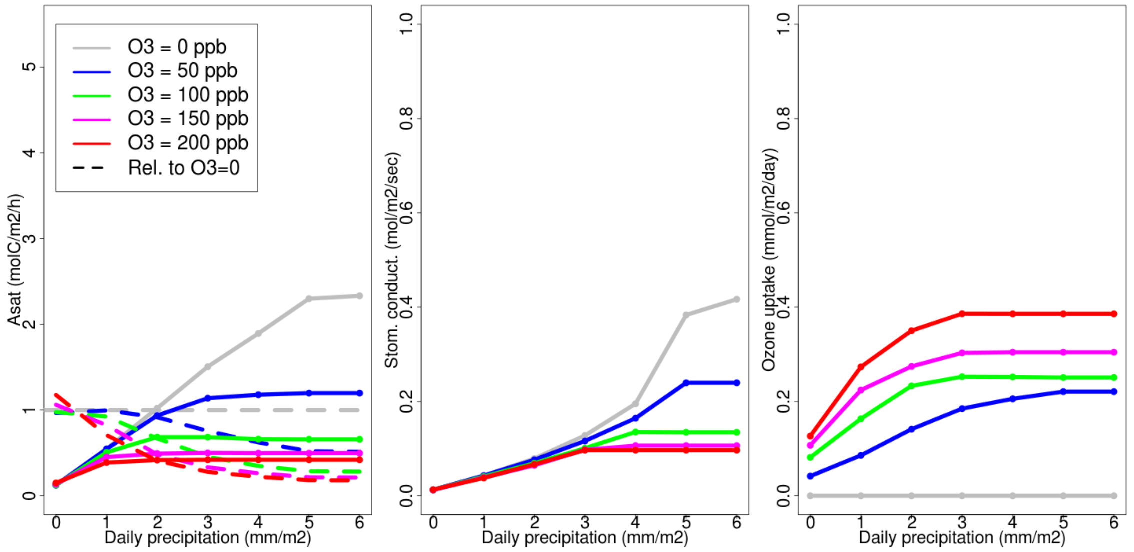
The response of three physiological parameters essential for yield formation is analyzed, in dependence of O_3 concentrations and one of CO_2 concentration, water provision or O_3 exposure time. Light-saturated photosynthesis (A_{sat}) increases with higher CO_2, but high O_3 concentrations dampen this increase. The relative loss in A_{sat} in reference to O_3-free conditions is, however, levelling off with higher CO_2. Stomatal conductance is reduced by a higher load of either CO_2 or O_3. At high O_3 and low CO_2 concentrations simulated stomata are completely closed. The influence of O_3 diminishes with higher CO_2 concentrations. Closely connected to stomatal conductance is O_3 uptake, which decreases with higher CO_2 but increases with higher O_3.

Scarcity of water leads to a less important role of O_3, evidenced by smaller differences between A_{sat}, conductance and O_3 uptake at low water levels. Both relative and absolute photosynthetic damages increase with water provision. For high O_3 loads stomatal conductance levels off: it does not increase with more water to avoid excess O_3 uptake.

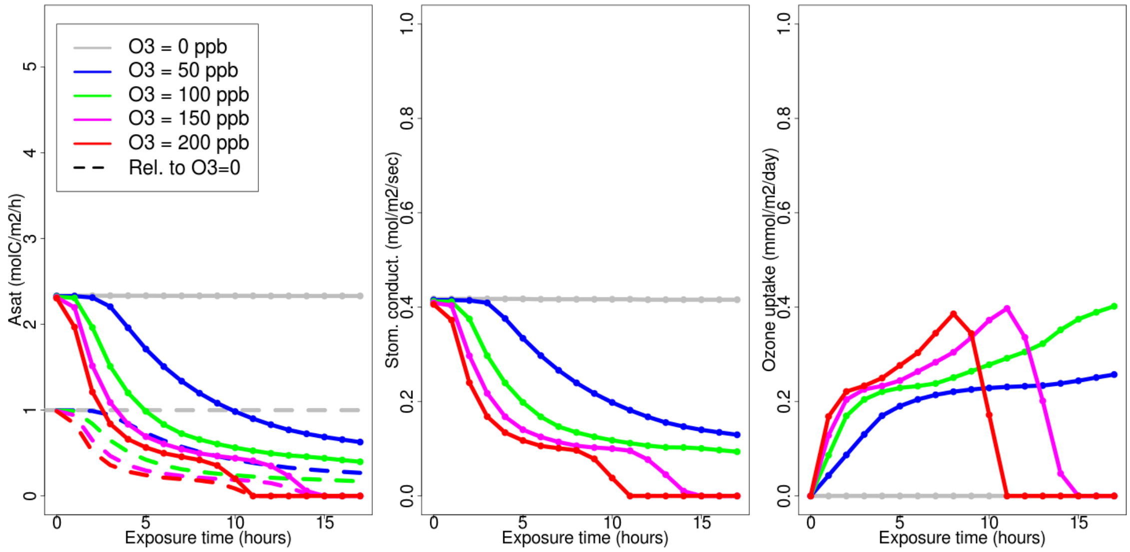
Longer O_3 exposure times lead to higher O_3 uptake and thus lower A_{sat} and stomatal conductance. Stomatal conductance, A_{sat} and O_3 uptake turn down to zero at high levels of O_3.



(a) Varying CO_2 concentrations, at 8 hours of exposure and 6mm daily precipitation



(b) Varying precipitation levels, at 8 hours of exposure and CO_2 at 340 ppm



(c) Varying exposure times, at 6mm daily precipitation and CO_2 at 340 ppm

***Figure 3**: Sensitivity of crop responses against varying inputs of CO_2 concentration **(a)**, water supply **(b)** and ozone exposure times **(c)** for Asian wheat. Data are taken as one-day snapshots at mid growing season (81 days after sowing) for Asian wheat. The response of A_{sat}, stomatal conductance and O_3 uptake is shown. Different colors denote different ozone concentrations.*

Model sensitivity towards varying ozone parameters, at constant weather and O_3 conditions, is shown in Figure 4. The five ozone-related parameters were varied between +/- 90% of their calibrated or fixed values. Simulated yields react most to changes in the detoxified fraction (d_{PFT}) of O_3: the more is detoxified, the higher are yield values. The second largest sensitivity is found towards senescence advancing (s_{PFT}); then follows the basal scavenging (bs_{PFT}). The Rubisco-limited photosynthesis penalty (j_{PFT}) shows impact only for Asian wheat, while the respiration increase factor (r_{PFT}) shows an influence only for soybeans. Sensitivities with parameters fixed at low, rather than mean, penalties are shown in SI Figure S7. These show distinct responses and orders of parameters, but underlining the choice of d_{PFT}, s_{PFT} and j_{PFT} as calibration parameters. Basal scavenging would exert measurable influence on yields, but was fixed as this is the only parameter that can be tied to literature values (see Methods).

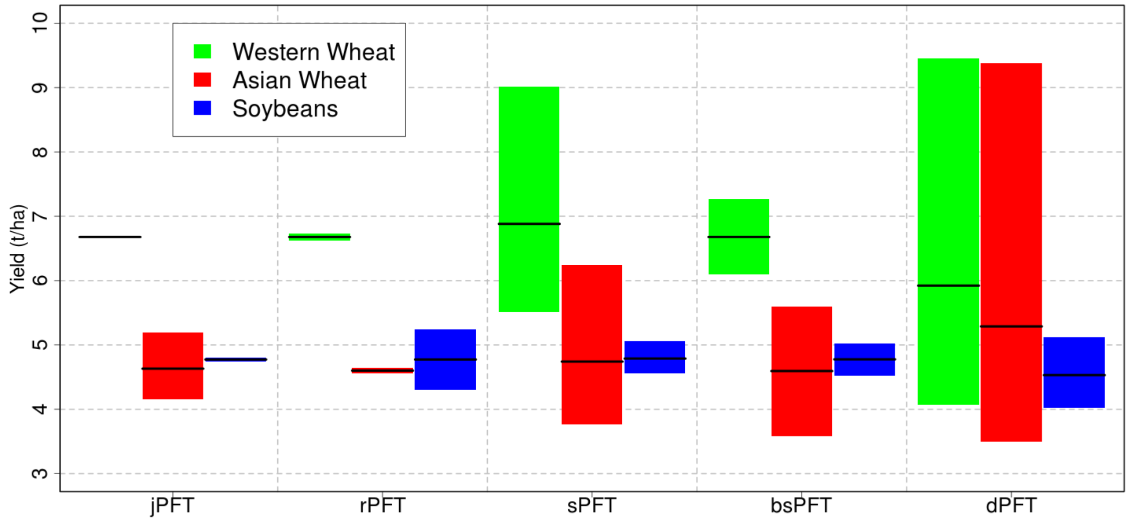


***Figure 4**: Sensitivity of simulated yields against perturbed crop parameters. Each of the five parameters was varied from -90% to +90% of its calibrated value (Table 2, except that dPFT was limited to a maximum of 100%); the other four parameters were held at their calibrated values. Black lines indicate mean yield values. Constant optimal temperature, precipitation and illumination were used (see SI Figure S7).*

Estimation of historical global yield losses

Historical global yield loss due to ozone pollution between 2001 and 2005 was calculated with LPJmL. Mean ozone levels during summer, based on the 'low' model ensemble, are displayed in Figure 5. These range from 7 ppbv in Amazonia and Papua-New Guinea up to 70 ppbv in the Middle East. Eastern US and Europe, in particular Italy, are stricken by high O_3 levels (40-60 ppbv) in the summer season. This suggests that major crop producing regions, which are mostly in the Northern Hemisphere, are substantially affected by O_3 pollution.

Maps of relative losses, separately for rainfed and irrigated yields, in comparison to a hypothetical scenario with zero surface ozone, are shown for Western wheat (Figure 6), Asian wheat (Figure 7) and soybeans (Figure 8). Both wheat types are simulated globally for comparison.

Irrigated yields show more pronounced relative losses (up to more than 50% wheat loss in highly polluted areas in Asia) than rainfed yields for all crops. Western wheat losses range from 0 to 20% for rainfed yields, with highest losses in Central Europe, followed by the Eastern US. Irrigated yield losses range between 5 and 25%, with low spatial variation within main producing areas. Globally, land-use weighted wheat losses were estimated at 2.9% for rainfed and 11.9% for irrigated yields, if all planted wheat was of Western type.

Asian wheat losses range between 0 and 25% for rainfed and 10-50% for irrigated crops. The highest losses occur in Pakistan and India, where ozone load is high and a substantial fraction of crops is irrigated. Major cropping areas in China also suffer from pronounced yield reductions due to ozone pollution. Abrupt changes between neighboring countries, for example Pakistan and Afghanistan, are largely due to different national management intensities (SI Figure S1). Globally, land-use weighted wheat losses were estimated at 7.3% for rainfed and 29.9% for irrigated yields, if all planted wheat was of Asian type.

Relative yield losses for soybeans are less substantial, ranging between 0 and 14% for rainfed crops, where the highest reductions are observed in Northern Italy and Northeastern China. The Northeastern US experiences ozone-induced soybean yield depressions of up to 10%. Reductions for irrigated soybeans are up to 15% in several regions, in particular in Northern China and the US Midwest. Globally, land-use weighted soybean losses are estimated at 3.8% for rainfed and 10.9% for irrigated yields.

Nationally aggregated yield losses due to ozone pollution are shown in Figure 9. Only the top producers (cumulatively accounting for at least 90% of global production between 2000 and 2011, split between Asian and Western wheat) for each crop are considered. Uncertainties in the estimation due to different O_3 inputs are shown by black lines. Mean losses for Western wheat range from 1% in Argentina, Australia or Canada up to 17-18% in Germany and the UK. For Asian wheat mean losses range from 13% in Iran and Egypt up to 46% in Pakistan. The large range is due to different management intensities and different matches of crop growing season and peak ozone load. Soybeans show mean losses between 0% in Argentina and 9% in China. For Argentina in some cases soybeans even gain yield with O_3 pollution, which is due to avoided water stress later in the season when phenology is advanced by ozone. The uncertainty range due to O_3 concentrations is around 22% of the mean loss, averaged over all crops and countries. Differences between countries are usually due to different levels of O_3 pollution, water limitation or management intensities, which affect canopy conductance. Calculations with a constant LAI_{max} of 5 for all crops and countries are shown in SI Figure S8.

Yield losses estimated with LPJmL were compared to two previous global assessments based on exposure-response functions. In Van Dingenen *et al.* (2009) and Avnery *et al.* (2011) the authors each compile a global ozone field for the year 2000, using a chemical model, and estimate yield losses with previously published ERFs for wheat and soybeans based on two different ozone damage indices. A comparison of the loss estimates is provided in Table 3. For LPJmL the mean of all ten ozone model inputs is supplied while for the ERF studies the mean from both indices is shown. Losses for soybeans are estimated consistently lower by LPJmL, with Africa as the only exception. Loss estimates for wheat deviate from the ERF studies, too, but not consistently.

Table 3*: Comparison of relative yield losses between previous estimates and LPJmL. For LPJmL Asian wheat parameters were applied in China, India and Northern Asia; all other regions use Western wheat parameters. Exact regional definitions can be found in the two ERF studies.*

Crop	**Region (Country)**	**Loss by ERF:** Van Dingenen *et al.* (2009)	**Loss by ERF:** Avnery *et al.* (2011)	**Loss by LPJmL**
Soybeans	North America	12.4%	14.4%	6.9%
	Latin America	n.a.	3.3%	2.4%
	Europe	23.9%	25.6%	14.8%
	Africa & Middle East	n.a.	5.9%	8.9%
	China / East Asia	16.1%	22.8%	8.8%
	India / South Asia	11.9%	8.2%	2.7%
	Oceania	n.a.	1.9%	1.1%
Wheat	North America	4.3%	6.8%	2.4%
	Latin America	n.a.	3.7%	0.8%
	Europe	4.4%	7.7%	8.2%
	Africa & Middle East	n.a.	13.0%	3.4%
	China / East Asia	14.4%	9.8%	11.1%

	India / South Asia	20.4%	17.4%	10.2%
	Northern Asia	n.a.	6.9%	2.6%
	Oceania	n.a.	0.5%	0.7%

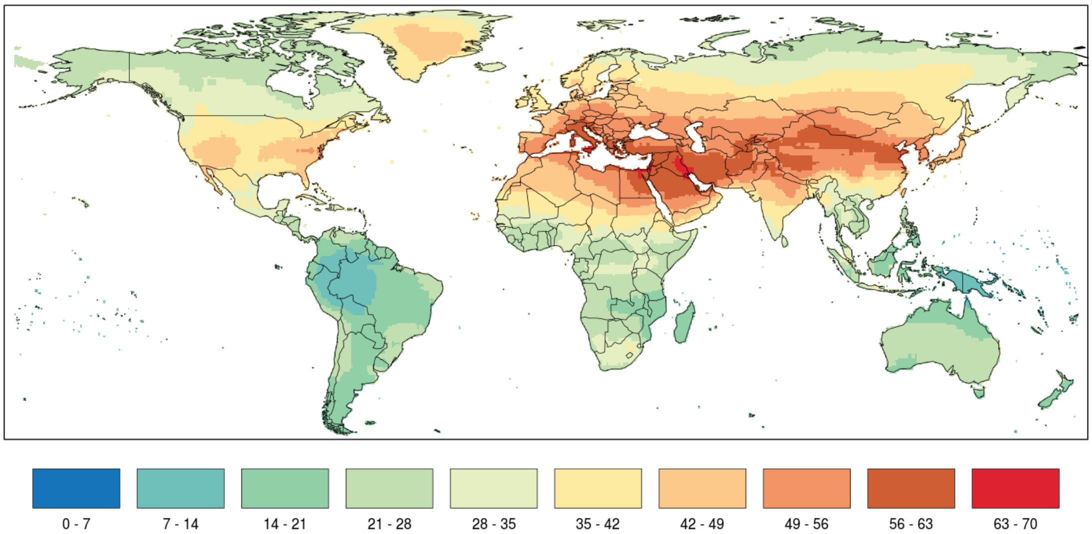
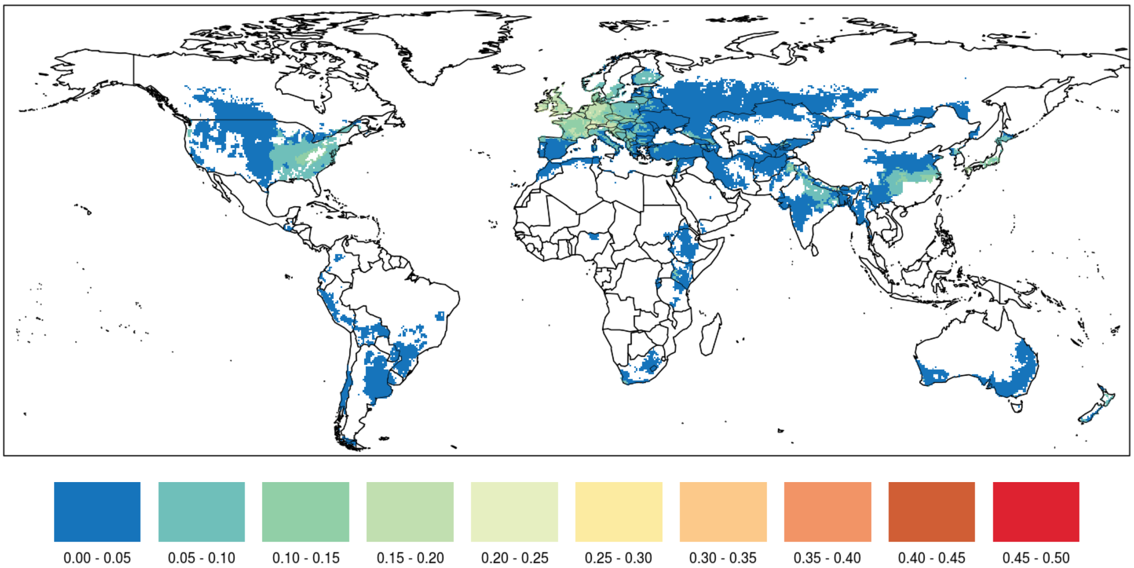
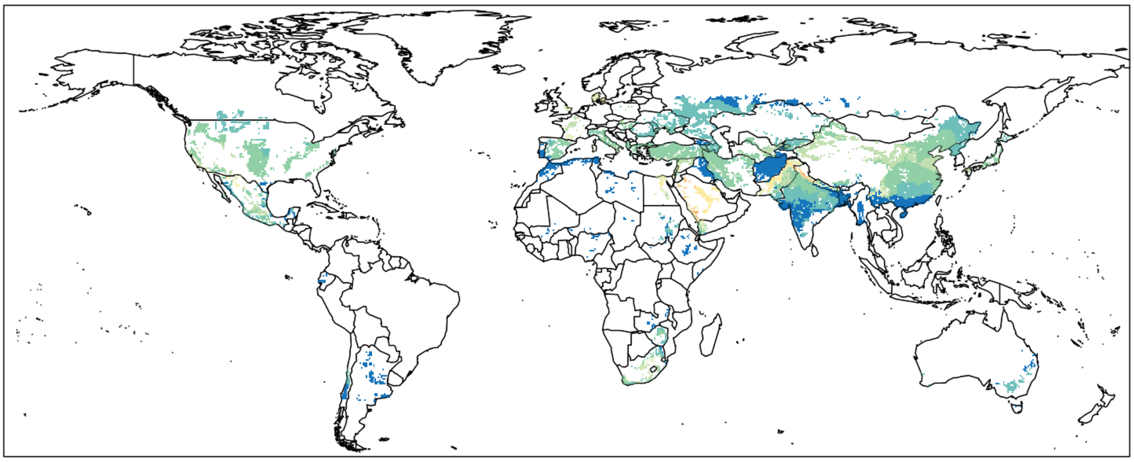


Figure 5: *Means of daily ozone levels in ppbv, averaged between 2001 and 2005 during the summer growing season, derived from the 'low' ensemble of ACCMIP models. Growing season is defined as April to August on the Northern and December to April on the Southern Hemisphere.*

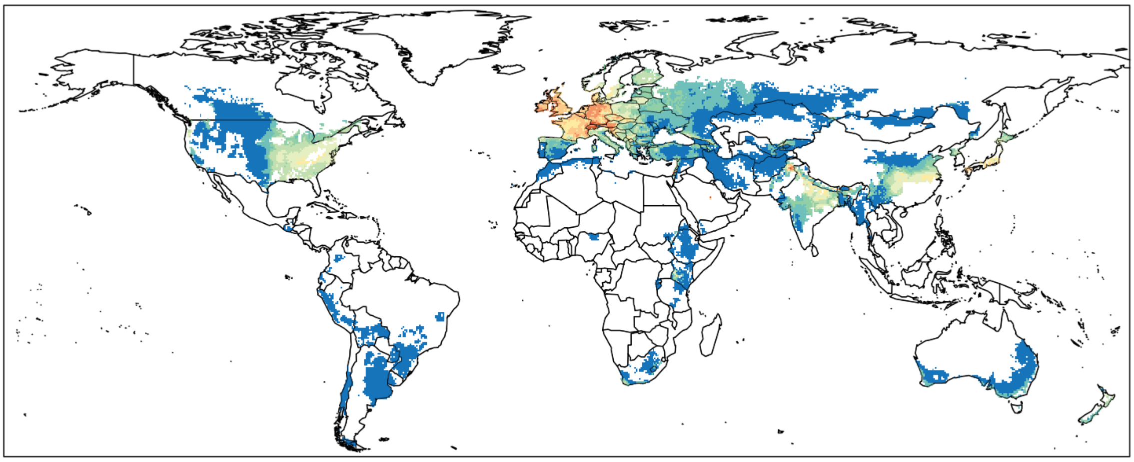


(a) Rainfed

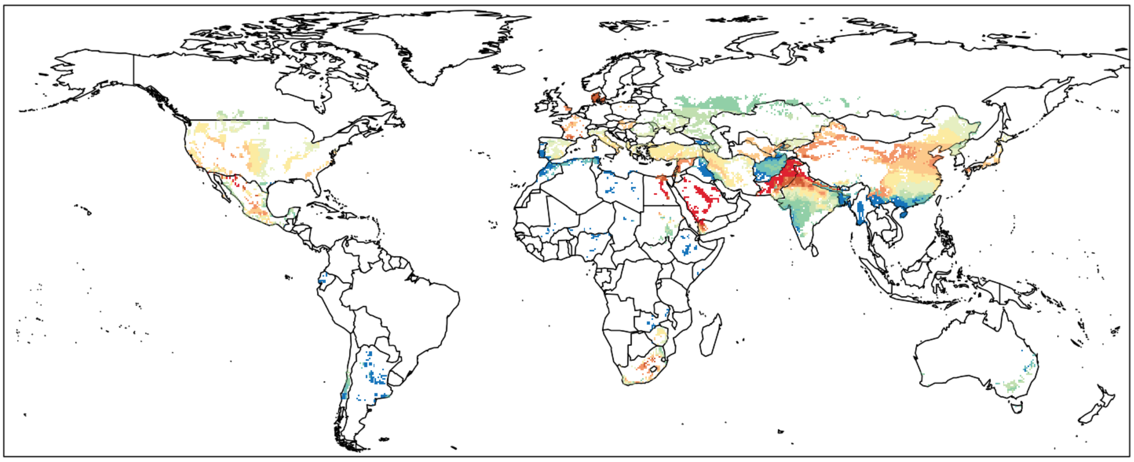


(b) Irrigated

Figure 6: *Historical Western wheat yield losses as fraction of unharmed yields at zero O_3. White areas have no cropping area in MIRCA2000. Panel* ***(a)*** *shows rainfed and* ***(b)*** *irrigated yields. The 'low' model ensemble was used as O_3 input.*

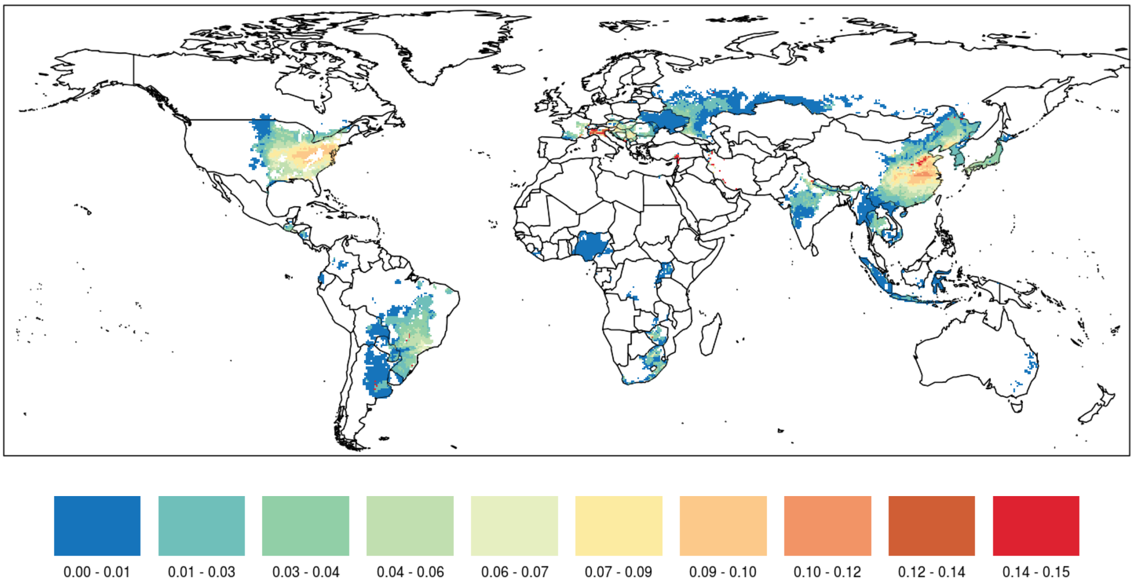


(a) Rainfed

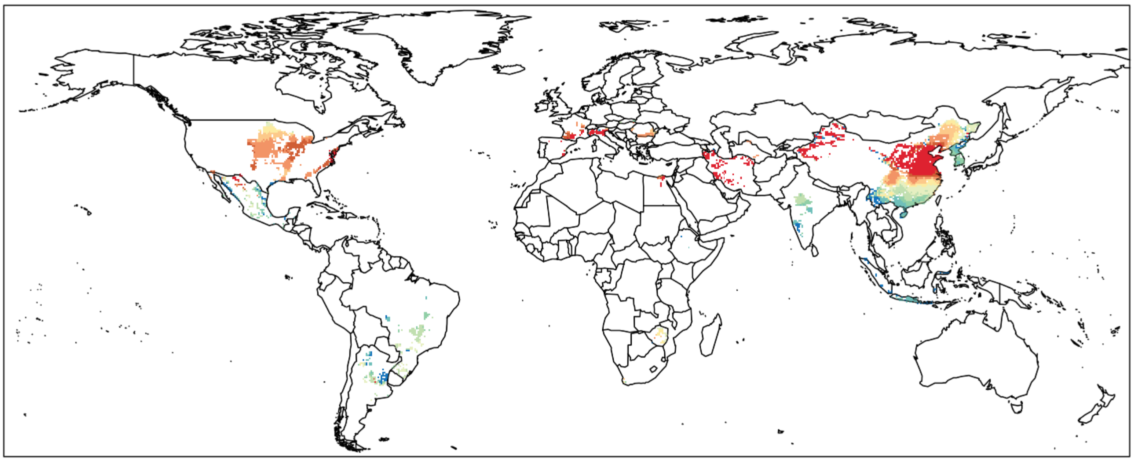


(b) Irrigated

Figure *7: As Figure 6, but for Asian wheat (same color scale).*

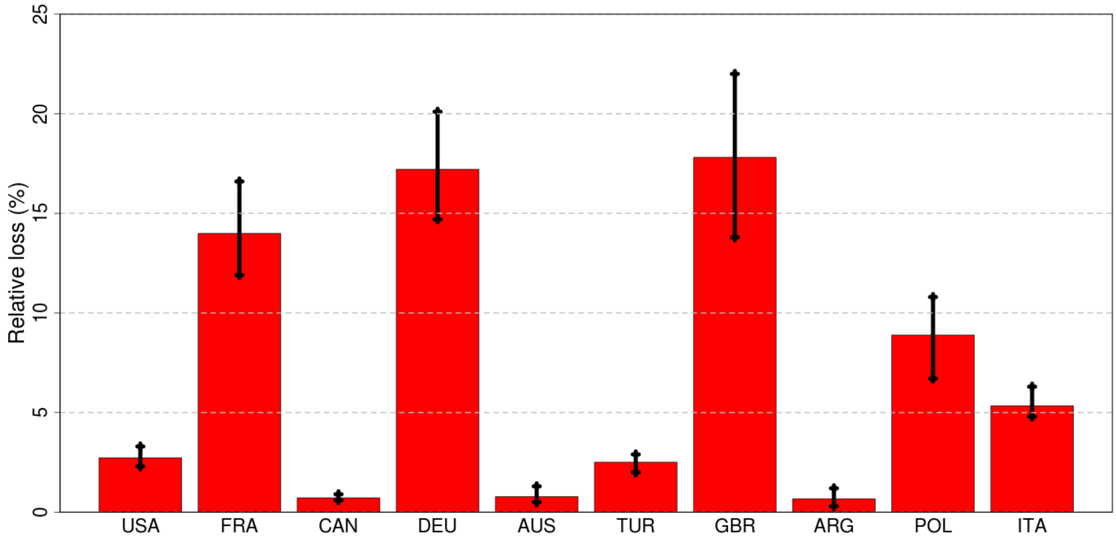


(a) Rainfed

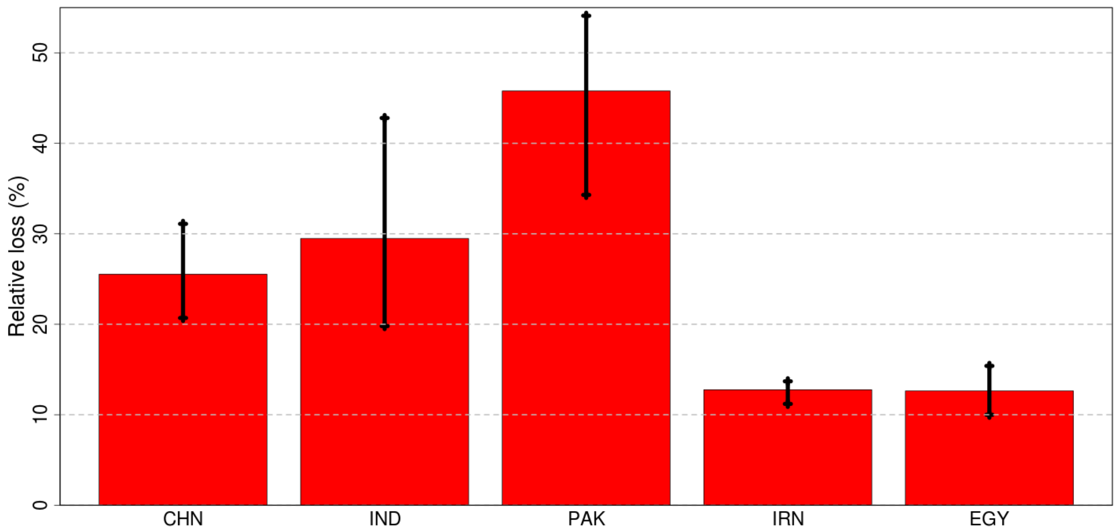


(b) Irrigated

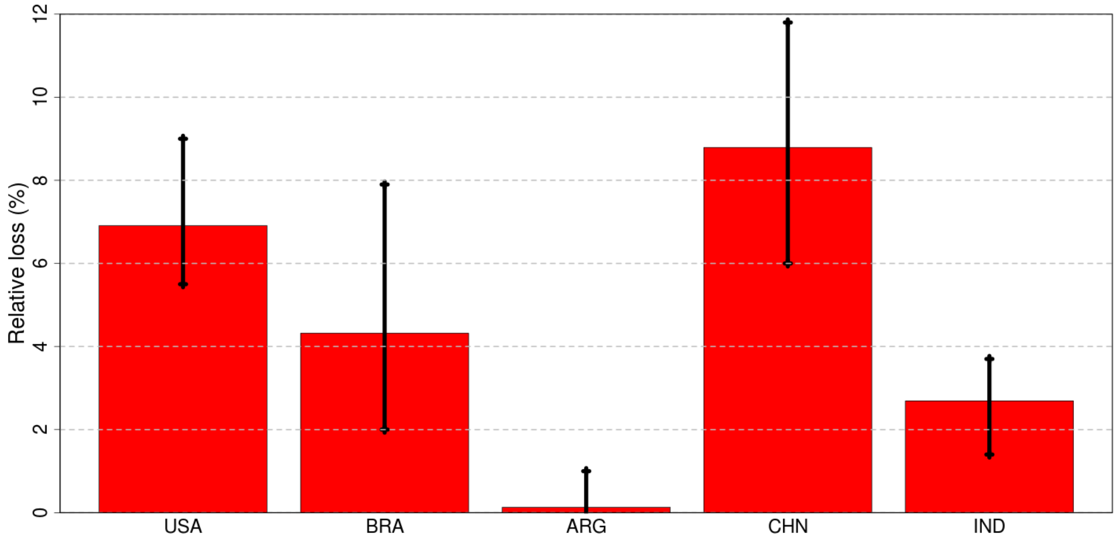
Figure 8: *As Figure 6, but for soybeans.*



(a) Western wheat



(b) Asian wheat



(c) Soybeans

Figure 9*: Nationally aggregated yield losses due to ozone, relative to zero pollution, for the main producers of each crop:* ***(a)*** *Western wheat,* ***(b)*** *Asian wheat,* ***(c)*** *soybeans. Red bars show yield losses as land-use weighted averages over all grid cells with at least 0.05% land-use share of the respective crop, as the mean of ten different global O_3 input fields. Black lines show loss ranges among them. Countries are ordered by total production.*

Discussion

We have implemented a novel ozone damage module into the widely used global crop model LPJmL. Parameters were calibrated to experiments and with these we have estimated global historical yield losses. Losses range from virtually 0% up to occasional 50% and agree with previous yield loss estimates in several cases. This study is the first to consider water stress, temperature, management intensity and CO_2 concentration as co-variates of ozone effects at the global level. To account for distinct sensitivities to O_3, Western and Asian wheat were simulated separately.

Model design

Simulating ozone damages with a process-based model is more complex than regressions between yield and accumulated pollutant exposure as in ERFs. But mechanistic descriptions offer several advantages: to capture non-linear effects on sub-seasonal scale, to account for variation in ozone response due to variable water supply or temperature and to include the antagonistic role of O_3 and CO_2. Our equation design, and also what was explicitly excluded, is based on a diverse literature background and was chosen for seamless integration into the LPJmL framework. Yet there are several caveats concerning the formulation. First, the advancement of phenology and senescence due to super-accumulation of heat units (only for soybeans) with ozone is not based on physiological knowledge. But the effect of O_3 on active LAI is captured with this approach, which was the main motivation in this study. Second, previous approaches implemented a decrease in photosynthesis from ozone by reducing V_{cmax}, the CO_2-limited maximum rate of carboxylation, as observed by experiments (Farage & Long, 1995). We chose to reduce the Rubisco-limited photosynthesis rate *jc* instead, as observed in Betzelberger *et al.* (2012), since respiration in LPJmL is linearly dependent on V_{cmax} and would therefore decrease with higher O_3 load. But this has not been observed in experiments – respiration increases with O_3 (Feng *et al.*, 2008). Third, LPJmL utilizes a big-leaf approach to scale from molecular processes to ecosystem level. This simplification neglects differential effects of O_3 on young and old leaves (Ewert & Porter, 2000), but is justified by the global scale as a necessary simplification. Fourth, a direct impact of O_3 on stomata apart from the coupling via photosynthesis effects (Lombardozzi *et al.*, 2012) is not considered since no data are available for crops. Fifth, the amount of ozone that is scavenged without any effect on the plant may change over time or in stressful conditions (Ewert & Porter, 2000, McGrath *et al.*, 2015). This is not considered due to lacking data on crops. Sixth, damage repair is not explicitly considered but subsumed with detoxification for the sake of model simplicity. This is inaccurate, though, since repair capacities diminish with leaf age (Ewert & Porter, 2000). Seventh, the daily time step may be too coarse to capture non-linear impacts of sub-daily ozone peaks. We account for this uncertainty by using two aggregations from hourly to daily O_3 concentrations (“low” and “high”) and by calibrating model parameters for daily time step simulations. Overall, we developed an ozone damage module of intermediate complexity that does not capture sub-daily, leaf-specific effects but runs globally and accounts for co-variates like temperature and water.

Parameter calibration and sensitivity

The high model sensitivity towards the detoxified fraction is due to its influence on all downstream processes (respiration, photosynthesis, senescence). Basal scavenging is an additive reduction and therefore does not show as large an influence as the respiration-driven detoxification d_{PFT}. Precocious senescence displays substantial influence on yields since it deprives the plant of radiation interception twice: less new leaves are formed and the existing ones are less active. The sensitivity towards parameters depends on crop and absolute parameter value. Therefore the parameters can only be interpreted as a complete set since they are dependent on each other and the rather few experimental observations do not seem to allow an unambiguous quantification of mechanisms. This suggests that possibly a more simple reduction of net photosynthesis by a combined penalty term would also be sufficient, as long as more experimental constraints are not available. Calibration seems to be more reliable for experiments that measure several considered target variables simultaneously (e.g. experiments 4 and 5 for soybeans) than for experiments with only few observed variables.

Though the dynamics of stomatal conductance are generally captured, there is a low bias for soybeans: simulated conductance for water is never above 0.7 mmol/m^2/sec, while measured values reach up to 1.2. This may impact ozone uptake and thus yield damage, resulting in a too low damage. But for the two experiments (Bou Jaoudé *et al.*, 2008) where measured conductance is largely underestimated by the model the measured values are unusually high even for perfectly illuminated and not water-stressed conditions in comparison to the other experiments. Additionally, experiments measure only the top leaves of the canopy. These are more conductive than lower leaves and therefore overestimate conductance under field conditions (Bernacchi *et al.*, 2007, Booker *et al.*, 2005, Bunce, 2004). We conclude that the underestimation by LPJmL is not systematic under field conditions, as the remaining experiments suggest. The conservative estimate of yield losses is equally explained by higher conductance under pot or chamber than under field conditions, for which LPJmL is designed. The close agreement between previous and our national soybean loss estimates indicates that this underestimation in experiments is not problematic under field conditions.

The usage of a global model with parameters that have been calibrated with point-based experiments may entail further uncertainties. This concerns management, weather or unobserved influences on yields that are not resolved at larger scales. We aimed to limit these uncertainties by using different types of experiments with varying locations and conditions. Experimental results should also be treated with caution since also among them there is uncertainty in the magnitude of ozone effects (Bernacchi *et al.*, 2006). Therefore it is reasonable to allow some error in the reproduction of experimental observations as long as these are unbiased and the dynamic range – large response differences from largely different conditions – is captured.

The association of predominant wheat type (Western or Asian) with country in our study is arbitrary and does not account for differences within each group. Additionally, except the ozone factors, all other crop parameters – which are derived from literature and intended to cover a broad range of wheat-type cereals like barley or rye – are kept constant, which may not reflect physiological reality. But the different values for ozone factors after calibration, with higher penalties for Asian wheat, and the agreement with previous studies of coherently larger losses in Asia support the geographical split into two types. Yet hypotheses about physiological reasons for the different response, e.g. a particularly sensitive photosynthesis in Asian types, cannot be deduced in the light of the current uncertainties.

Sensitivity towards input data

Simulated responses to different climate conditions agree with expectations. The antagonistic roles of O_3 and CO_2 (Bernacchi *et al.*, 2006, Ewert & Porter, 2000) and the protective role of water deficit against O_3 damage (at the price of generally lower yields) are captured. Higher ozone loads or longer exposure also lead to more damage, as expected.

Absolute and relative yield losses are dependent on management intensity. Management including fertilizer, cultivar choice or pest control is reflected only by the parameterized maximum leaf area index (LAI_{max}) in LPJmL (Fader *et al.*, 2010), since the utilized version does not contain explicit nitrogen cycles or pest dynamics. A LAI_{max} of 5 (maximum is 7) for Germany and the UK is also the reason for unexpectedly high losses of 17-18%. Therefore the correct adjustment of management in the model is of salient importance. LAI_{max} was separately scaled for each country and crop, at zero ozone concentration, between 1 and 7 such that national mean yield levels between 1998 and 2002 match between LPJmL simulations and FAO reported yields (FAO, 2016). Calibrated LAI_{max} values may therefore contain implicit ozone damage, in particular in countries like India or Pakistan, where FAO yields are clearly depressed by ozone which is not reflected in LPJmL at zero O_3. An O_3-sensitive calibration will have to be done in the future. Experimental evidence, meanwhile, also suggests that a scaling of losses with better management is reasonable, in particular when leading to higher stomatal conductance (Biswas *et al.*, 2008).

Reliability of ozone input data

We compared monthly ozone data, derived from hourly ozone concentrations from four ACCMIP models, to the observational data set provided by Sofen *et al.* (2016); see SI Figure S3. Both 'low' and 'high' ensembles tend to overestimate low monthly ozone pollution, in particular in northern latitudes. Reasons for this bias are discussed in Fiore *et al.* (2009) and Schnell *et al.* (2015). A local-mean-based bias correction was attempted for our study, but did not alter results much (data not shown). The existing uncertainties in ozone modeling require more sophisticated methods for correction, which we did not aim for in this study. A study on pollution-related mortality (Fang *et al.*, 2013) used ozone inputs with a similar bias as our ensemble. Therefore we used the uncorrected single models and ensemble, assuming to cover uncertainties regarding ozone input by using four different models plus their ensemble.

Ozone input was assumed as static in our study, i.e. daily concentrations are not modified by uptake or dry deposition. An atmospheric coupling between transpiration, vapor pressure deficit and uptake of CO_2 or O_3 would be necessary to capture the full dynamics of this complex process. This is currently not included in any crop model and requires interaction between biosphere and atmosphere models. Thus we assume static ozone fields as sufficient to assess national yield losses due to ozone.

Comparison to previous loss estimates

Our loss estimates for rainfed soybeans compare well with previous results. The LPJmL-based loss estimate for total US soybeans is 6.9% (range is 5.5 to 9.0%). For only rainfed yields this figure is 6.8% (5.3-9.0%), and for only irrigated yields 12.8% (11.3-14.6%). The value estimated by LPJmL is therefore close to the value of 5.5% for rainfed US soybeans provided by McGrath *et al.* (2015). Indian yield loss estimates by LPJmL are 2.7% (1.4-3.7%) for soybeans, corresponding exactly with the 2.7% (+/- 1.9%) estimated by Ghude *et al.* (2014). For Indian wheat a loss range agreement is found between LPJmL with 29.5% (19.8-

42.8%) and the study by Burney and Ramanathan (2014), who estimate 40% (20-60%, depending on the state). Note that, due to multicollinearity and data scarcity, Burney and Ramanathan (2014) consider black carbon and ozone together and do not feed concentrations but rather precursor emissions into their equations. Therefore estimates are not directly comparable. But loss calculations in Ghude *et al.* (2014) are more than five-fold lower with 5.0% (+/- 1.2%). In that study, the region most affected by ozone is estimated to suffer from 17% yield loss, which is just short of the lowest (national) loss estimate by LPJmL of 19.8%. A possible reason for differences is water stress: LPJmL explicitly simulates the interaction of water and ozone, while most statistical studies use a linear relationship between ozone and yields under all circumstances. A precipitation control is included in McGrath *et al.* (2015) and Burney and Ramanathan (2014), but not Ghude *et al.* (2014). This may explain the difference for wheat, which is mostly irrigated in India, and the match for soybeans, which are mostly rainfed in India. Therefore we conclude that the consideration of water availability is of pristine importance when assessing ozone losses. This may entail an economic trade-off for irrigation at the end of the season when ozone load is high: more irrigation also leads to more ozone damage, such that the cost for irrigation may just be leveled by the costs for ozone damage. This relationship has to be studied in more detail, though.

Our loss estimates agree to some extent (Table 3) with the global studies by Avnery *et al.* (2011) and Van Dingenen *et al.* (2009). Possible reasons for differences are divergences in ozone concentration due to different chemistry models, the consideration of only one year (2000), no distinction between Asian and Western wheat types and, above all, the lack of water levels in their ozone response. This may lead, as above, to overestimation of losses in water-stressed regions but to an underestimation in well-watered regions. Other putative causes for differences include a possible error in the growing season simulated by LPJmL, a wrong adjustment of management settings with LAI_{max} or temperature effects on crops. The effect of LAI_{max} is, however, limited as losses from crop/country-specific LAI_{max} values (Figure 9) are similar to losses at a constant high management (SI Figure S8). In our assessment and the statistical estimates a baseline of zero O_3 was used for comparison. This is unrealistic in practice since background biogenic emission of precursors cannot be mitigated. A more realistic estimate of *avoidable* ozone damage could therefore use a comparison level of, for example, 35 ppb, just below the AOT40 threshold.

Historical loss estimations

The estimation of historical yield losses due to ozone pollution suggests that ozone is a major yield-reducing factor in several regions on the globe. This agrees with expectations founded on experimental findings and observed ozone pollution. Reduction in the field is usually less than in chambers, at equal O_3 concentration, due to protective effects of water status (Fuhrer, 1995), sub-daily timing (Heath *et al.*, 2009), though not reflected in LPJmL, and a possible shift between growing season and peak ozone load, depending on crop and region (Van Dingenen *et al.*, 2009).

Asian countries are simulated as particularly susceptible to losses for two reasons: higher pollution and higher sensitivity of crops (Emberson *et al.*, 2009). The high loss estimation of more than 40% for wheat in Pakistan can be explained by these two factors and an almost exclusively irrigated cultivation, which allows for stomata to stay open and for more ozone to enter. It may, though, be too high an estimate given the sensitivity of the model towards management intensity and the uncertainty of ozone input data with very few observations in this region. Additionally, our simulations assume near-perfect potential irrigation without limitations due to water availability – which may not be realistic. Rather high reductions of 14-18% for wheat in France, Germany and UK wheat are unexpected, but may be reasonable in the light of substantial ozone pollution, limited water stress and high management intensity. Another factor is the possible overestimation of ozone pollution in Western Europe by the model ensemble (SI Figure S3). Loss estimates using only the GEOSCCM model, whose ozone concentration estimates match better with observations in Western Europe (data not shown), are lower (12-15%).

LPJmL estimates relative yield losses from irrigated yields as consistently higher than from rainfed yields. This is due to a higher stomatal conductance allowing more ozone to penetrate. Several experiments have shown this relative protective effect of water deficit (Bou Jaoudé *et al.*, 2008, Fuhrer, 1995, Khan & Soja, 2003). In McGrath *et al.* (2015), however, the authors find the opposite for rainfed soybeans in the US: losses are higher under dry conditions. They argue for a decoupling of stomatal conductance and water status by impaired abscisic acid (ABA) signaling. This eventually allows more ozone to enter under drought than under unstressed conditions, which aggravates losses. Another possible explanation for their finding could be that water-stressed plants have a limited capacity to detoxify ozone as antioxidant compounds are also necessary to combat drought consequences. Since neither model is currently able to resolve these processes, more detailed models and experimental studies are necessary to identify them.

Further model developments could comprise the inclusion of C_4 crops like maize, the combination of O_3 effects with other pollutants like SO_2 or NO_2 (Rai *et al.*, 2007) or the usage of different cultivars and sensitivities. Further questions that can be answered are adaptation options (e.g. shifting growing season, using different cultivars, ozone-sensitive water management) or assessment of future losses due to O_3. A coupled modelling between atmosphere, chemistry and biosphere would additionally allow for assessing the effects of mitigation more realistically.

Our implementation of a process-based global model to estimate historical yield losses from ozone has confirmed previous findings: major crop producers suffer from substantial production damage due to ozone pollution. This is a clear indication that more efforts to emit precursor emissions entail double benefits: less yield reductions and less health problems. Our research has emphasized that damaging effects are dependent on cofactors, in particular water status, which should be considered when establishing O_3 pollution thresholds. We consequently consider the inclusion of O_3 effects on crops as relevant for climate change impact studies, as climate change can alter water cycles, temperatures and ozone pollution. This would lead to modified yield expectations, with modifications possibly in a similar range as current uncertainties of crop projections (Rosenzweig *et al.*, 2014).

Two corollaries can be drawn from our assessment: first, establishing more surface ozone observation stations in particular in Asia, Africa and Latin America, as these regions are currently data scarce (Sofen *et al.*, 2016) but suffer from ozone damage and, second, documenting all conditions (ozone, temperature, water etc.) and results (yield, stomatal conductance, photosynthesis, respiration) in experimental studies to allow for a more stringent evaluation and parameterization of models.

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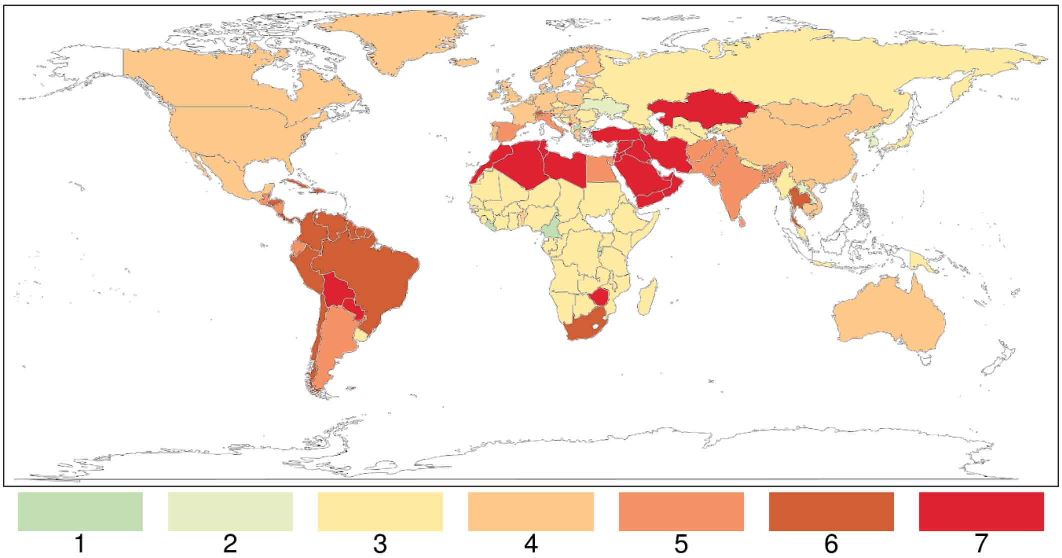
3.2 Supplementary Information

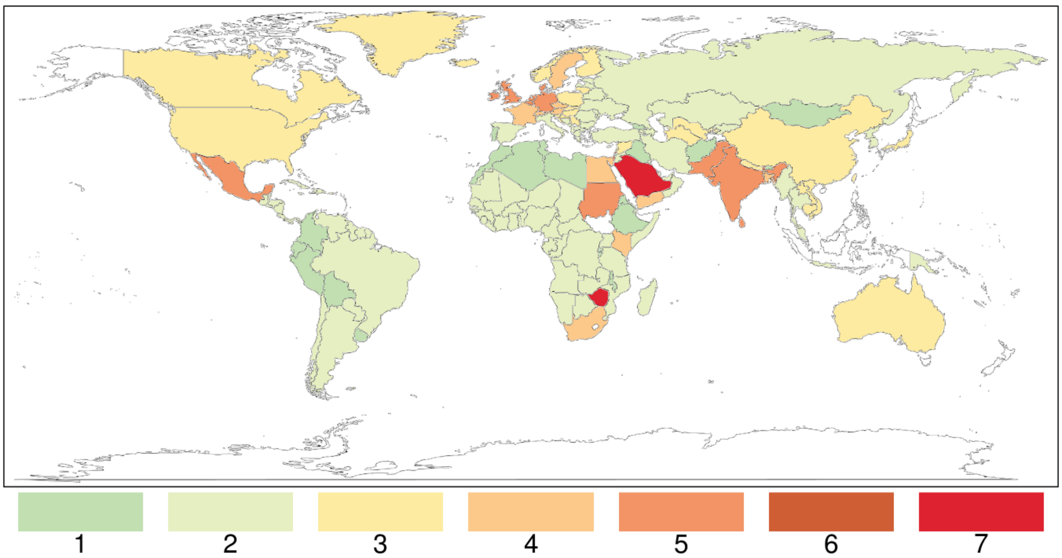
Supplementary information to "Global historical soybean and wheat yield loss estimates from ozone pollution considering water and temperature as modifying effects"

B. Schauberger, S. Rolinski, S. Schaphoff, C. Müller

Supplementary Figures



(a) Soybeans



(b) Wheat

***Figure S1**: World maps of management adjustment settings, as LAImax, for **(a)** Soybeans and **(b)** Wheat. Western and Asian wheat are not distinguished here. Note that the definition of a LAImax for a country does not indicate that this crop is actually grown there.*

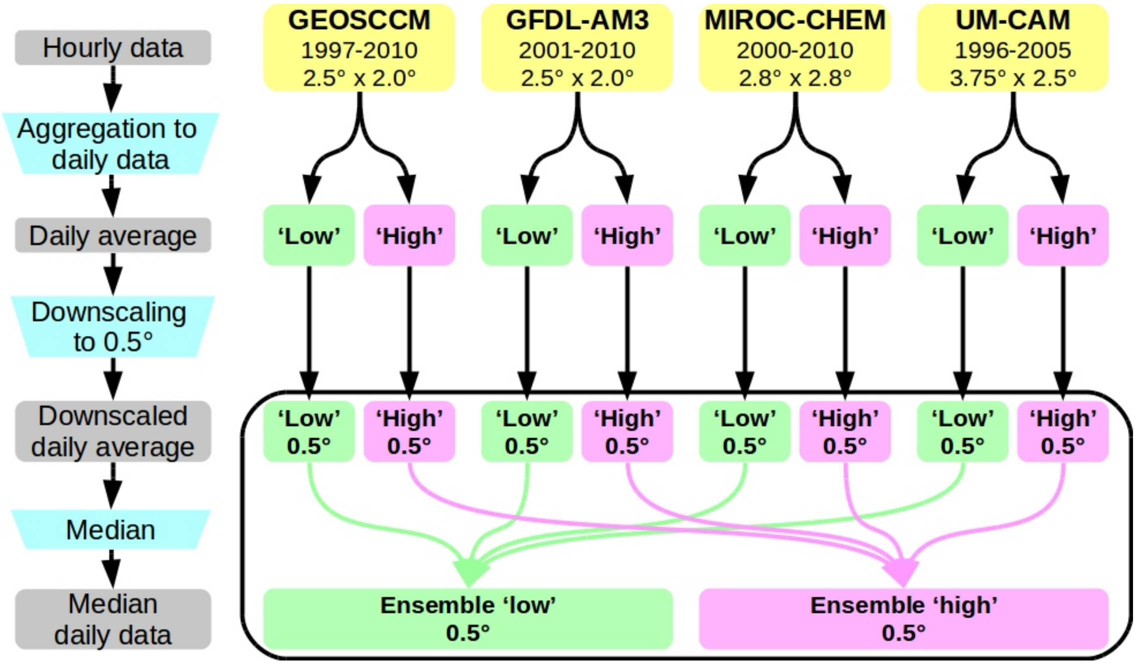


Figure S2: *Workflow for the preparation of global daily ozone input fields. Hourly data from the four global chemical transport models (yellow boxes) are aggregated to daily values by calculating the weighted mean between the daily mean and maximum hourly values for each grid cell. For the 'low' aggregation, the mean is assigned double weight while for the 'high' aggregation the maximum concentration during the day is assigned double weight. These daily values are then downscaled from the model resolution to 0.5° with a double conservative remapping (conserving fluxes and spatial gradients). The downscaled daily values are combined into two distinct ensembles, one from the 'low' and one from the 'high' daily aggregates. This results in ten different daily gridded ozone fields (marked by the black rounded rectangle).*

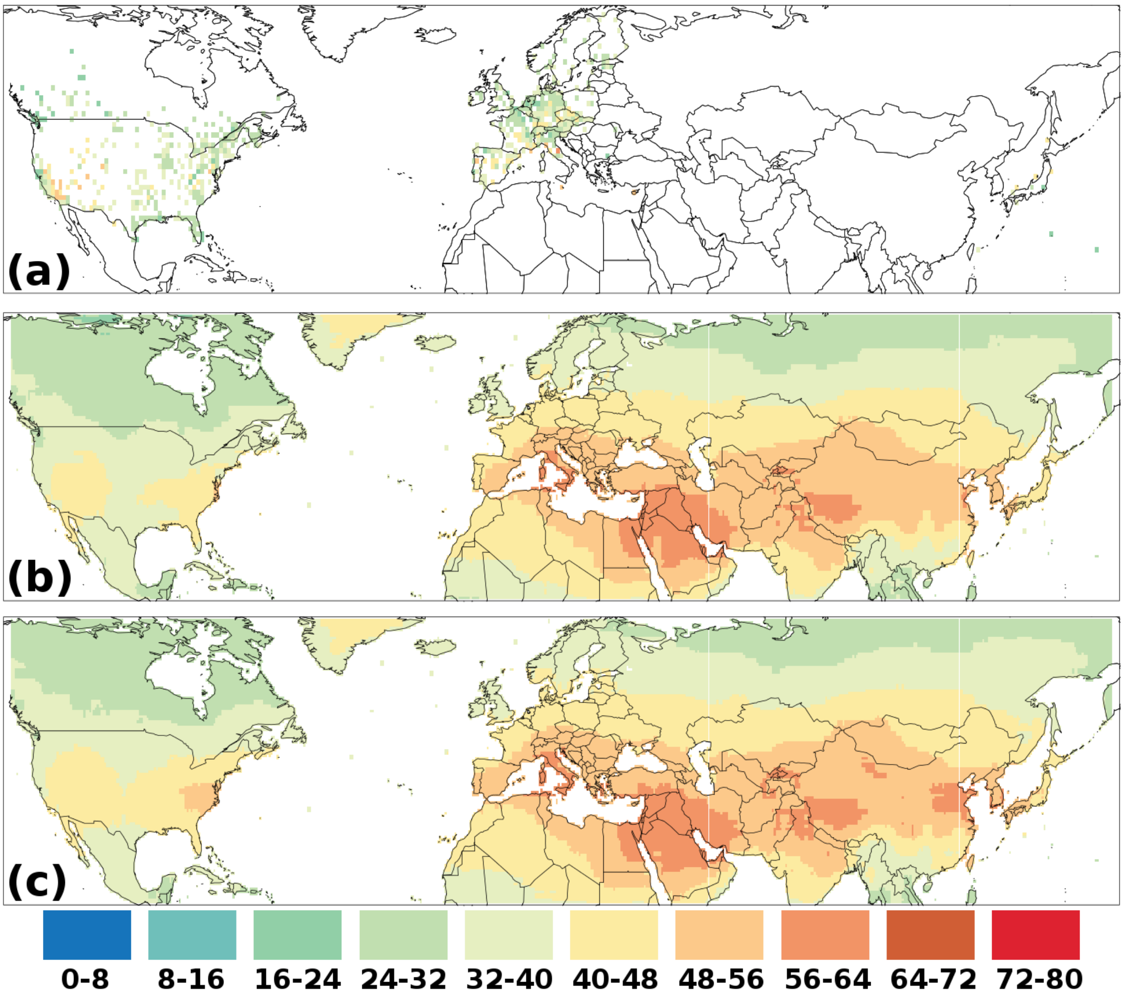
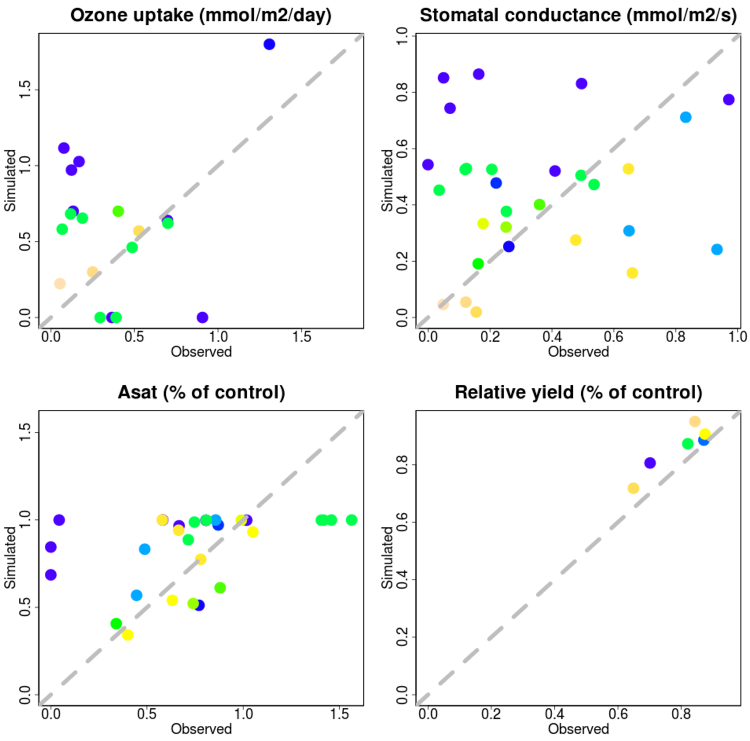
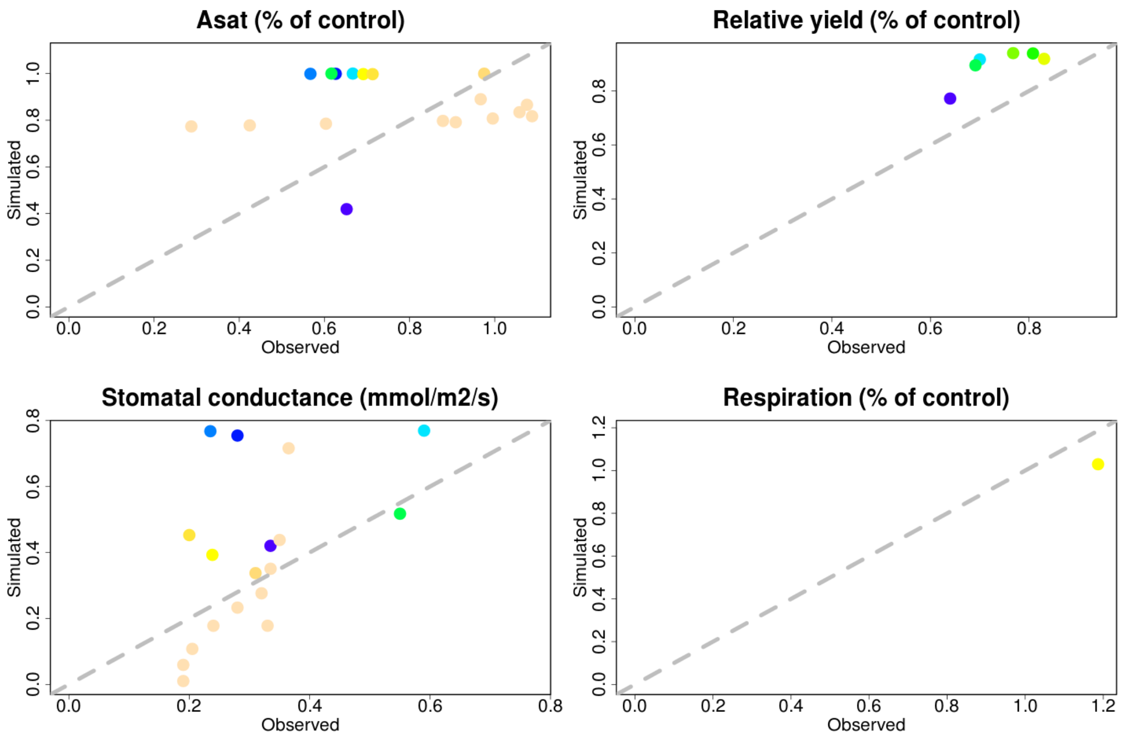


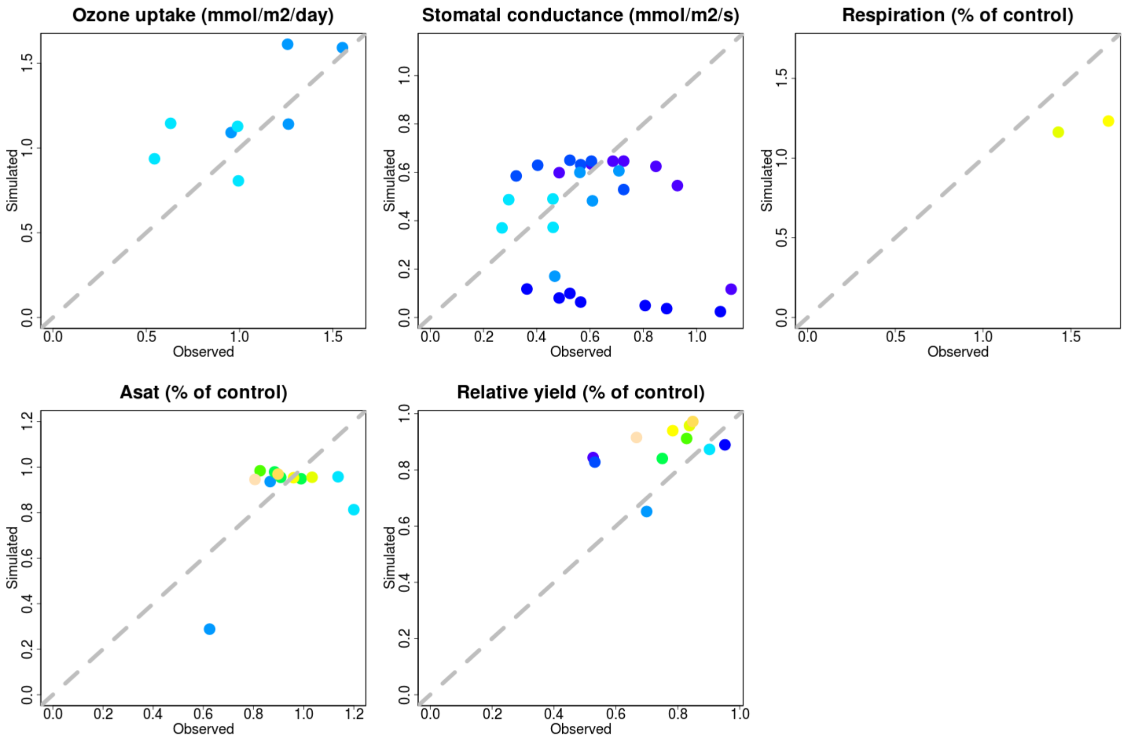
Figure S3: *Comparison of modeled* ***(b, c)*** *and observed* ***(a)*** *surface ozone concentrations. Observed data are provided by Sofen et al. (2016), while modeled data are represented by the 'low' (b) and 'high' (c) ensembles of four global chemical transport models. All data are monthly medians of hourly observed values, averaged over the years 2001-2005. Only the map section with available observed data is shown.*



(a) Western wheat

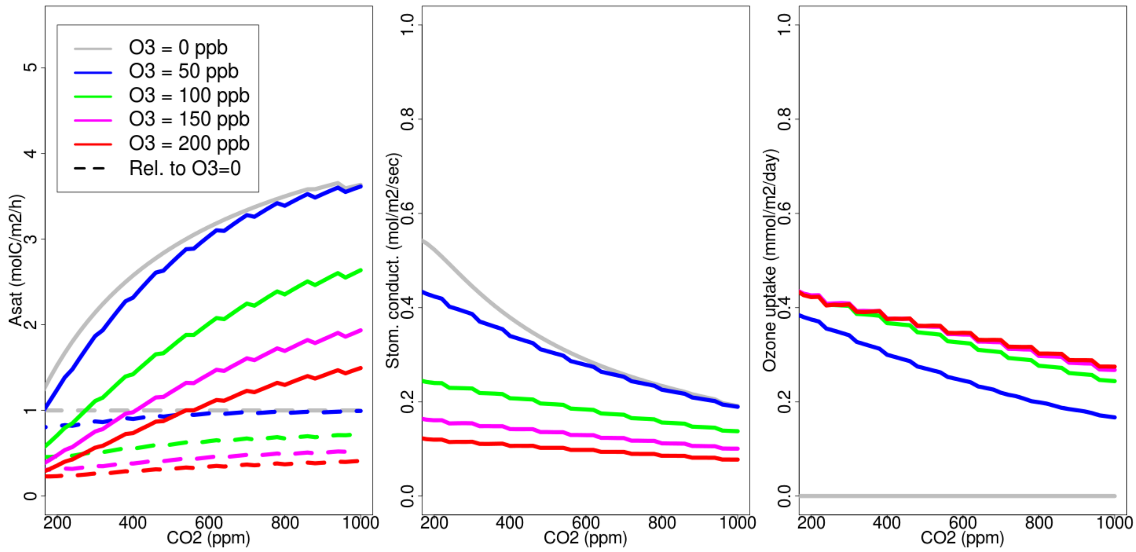


(b) Asian wheat

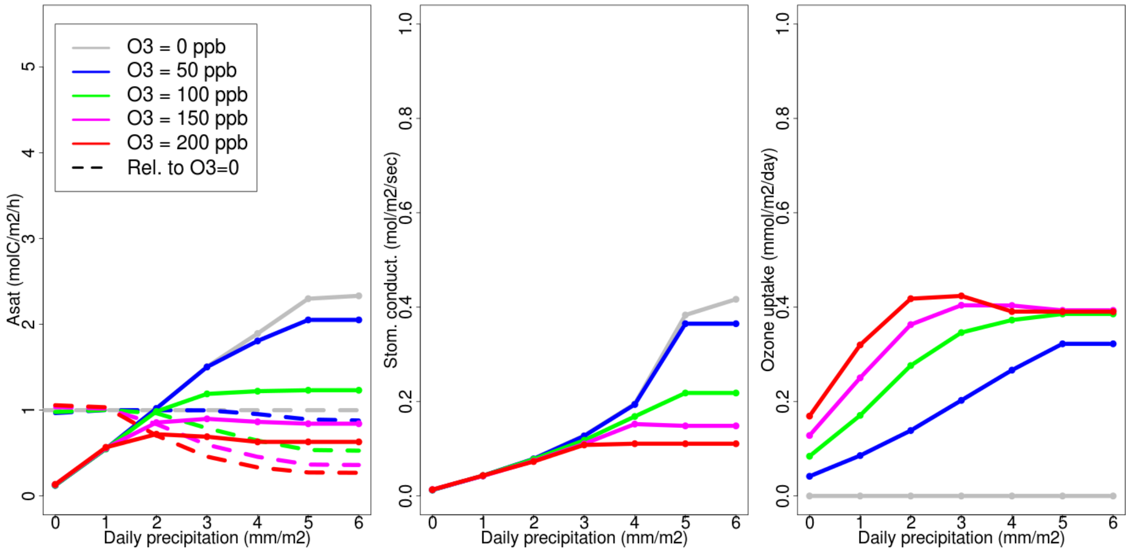


(c) Soybeans

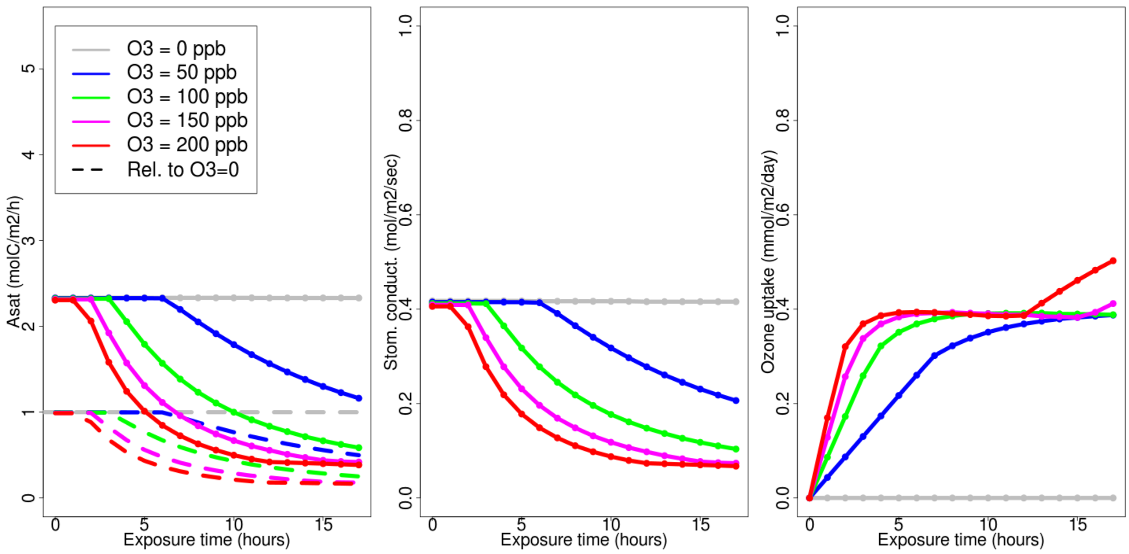
Figure S4: *Out-of-sample calibration results for **(a)** Western wheat, **(b)** Asian wheat and **(c)** Soybeans. Each experiment was omitted from calibration in turn; afterwards simulated results for this experiment – using the parameters calibrated only from the other experiments – are compared to observed values. These comparisons are shown here.*



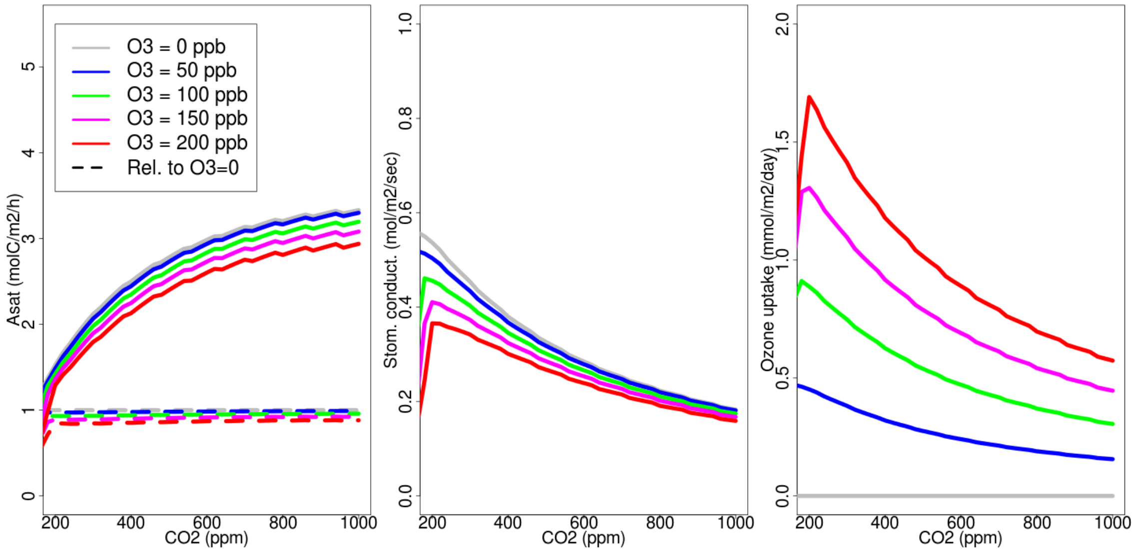
(a) Western wheat: Varying CO2 concentration



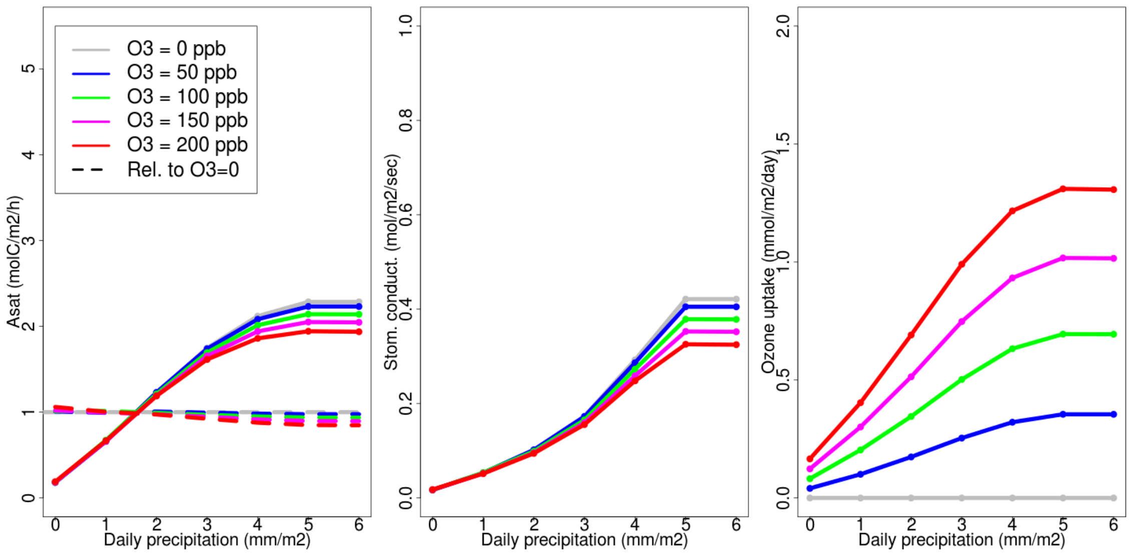
(b) Western wheat: Varying precipitation



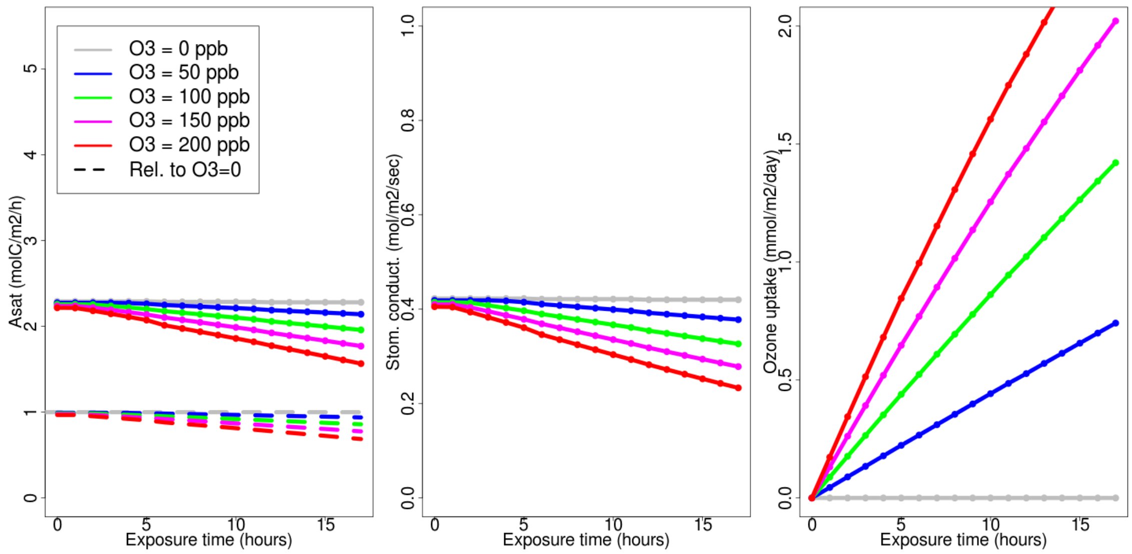
(c) Western wheat: Varying ozone exposure times



(d) Soybeans: Varying CO2 concentration

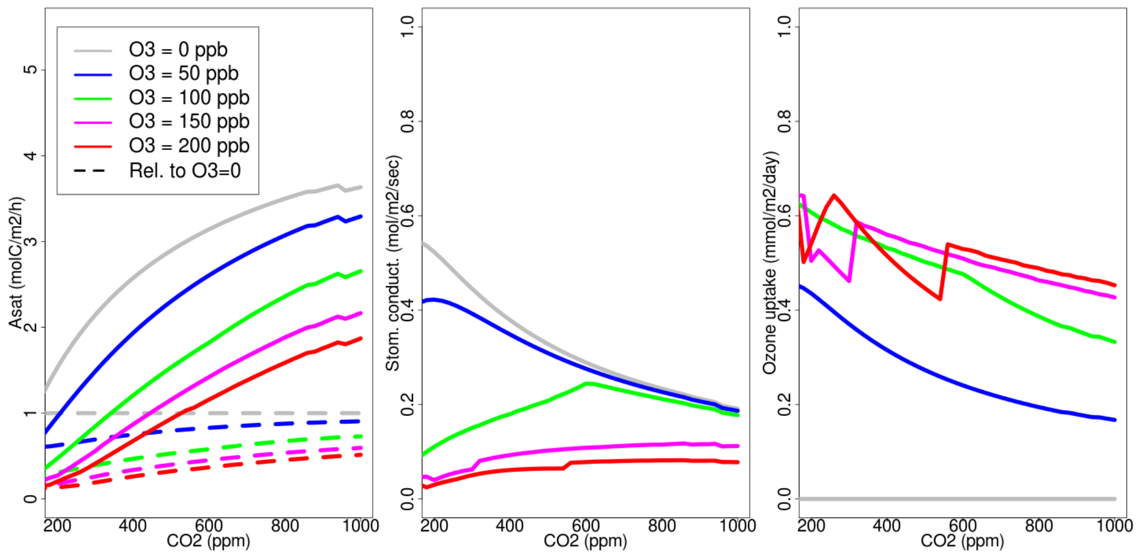


(e) Soybeans: Varying precipitation

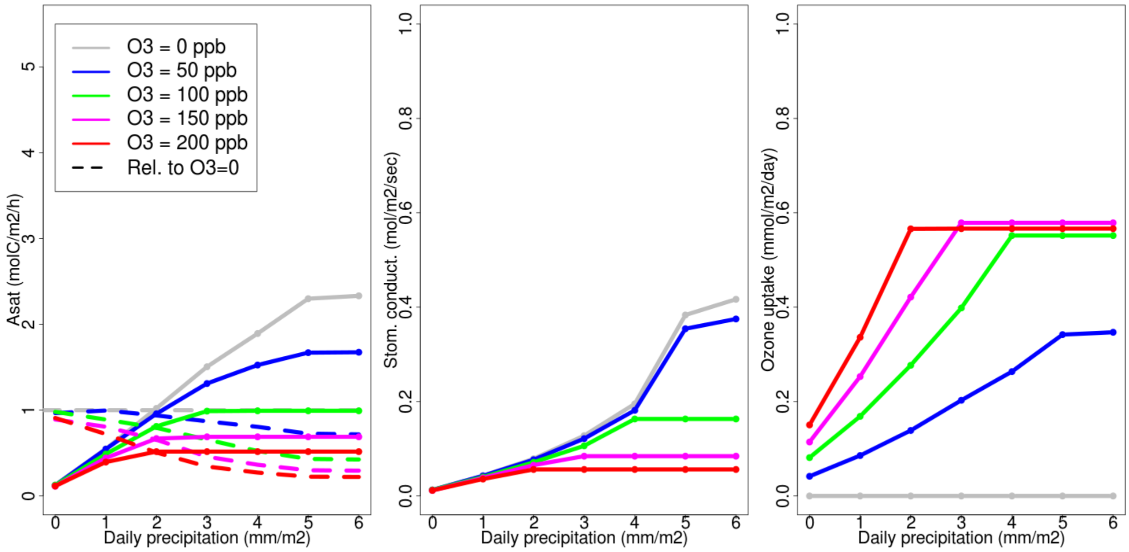


(f) Soybeans: Varying ozone exposure times

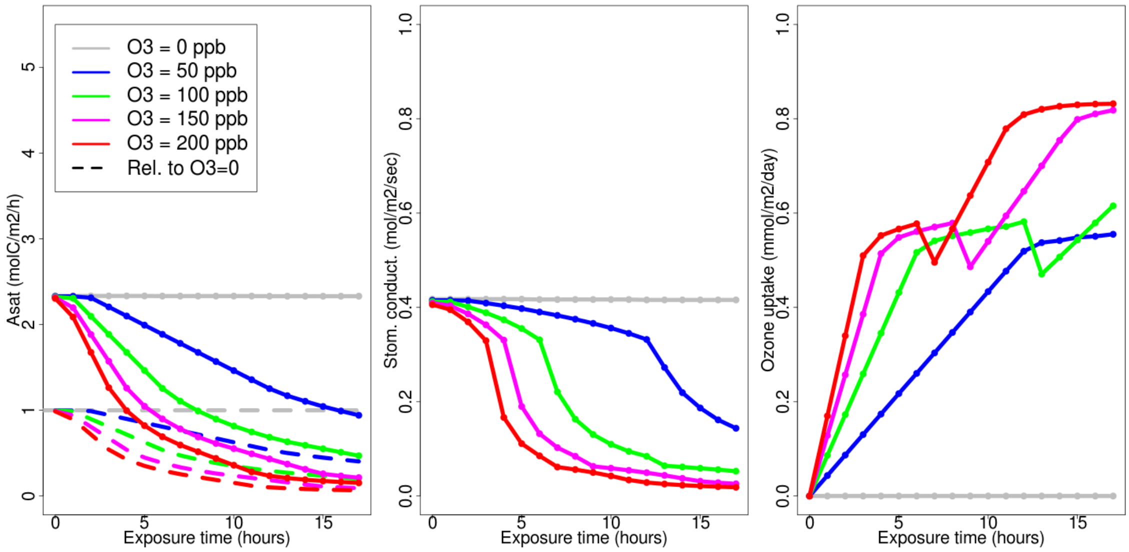
Figure S5*: Similar to Figure 3 in the main paper, but for Western wheat* ***(a-c)*** *and soybeans* ***(d-f)****. All other settings are equal as described for Figure 3.*



(a) Varying CO_2 concentrations, at 8 hours of exposure and 6mm daily precipitation



(b) Varying precipitation levels, at 8 hours of exposure and CO_2 at 340 ppm



(c) Varying exposure times, at 6mm daily precipitation and CO_2 at 340 ppm

Figure S6*: Similar to Figure 3 in the main paper these are sensitivity runs against varying inputs, as one-day snapshots taken at mid growing season (81 days after sowing) for Asian wheat. In contrast to Figure 3, the senescence advance with accumulated O3 uptake is switched off, allowing do detect pure ozone effects without mixing with LAI effects. The response of Asat, stomatal conductance and O_3 uptake is shown, varying with CO_2 level (panel* ***a****), water supply* ***(b)*** *and ozone exposure times* ***(c)****.*

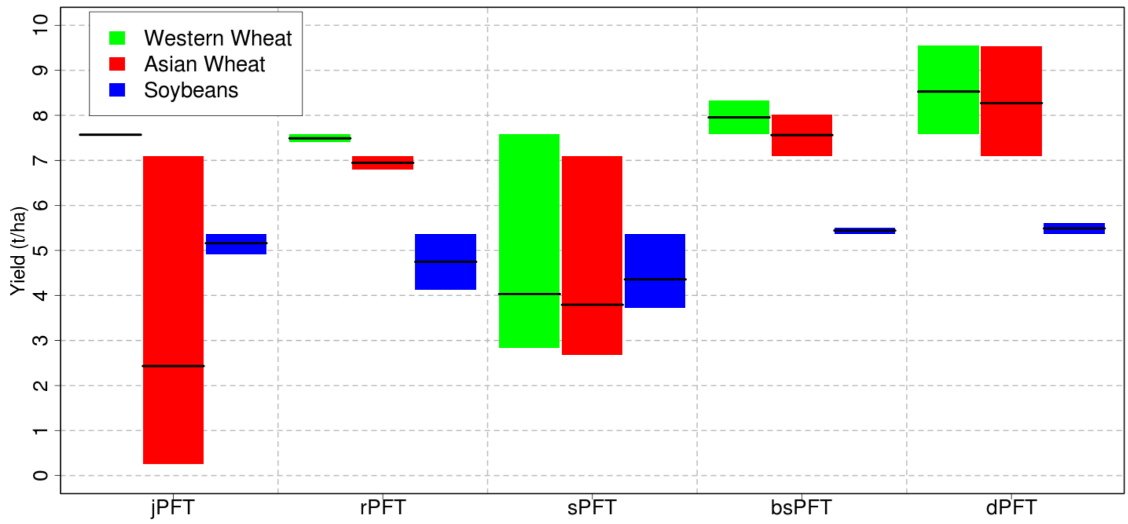
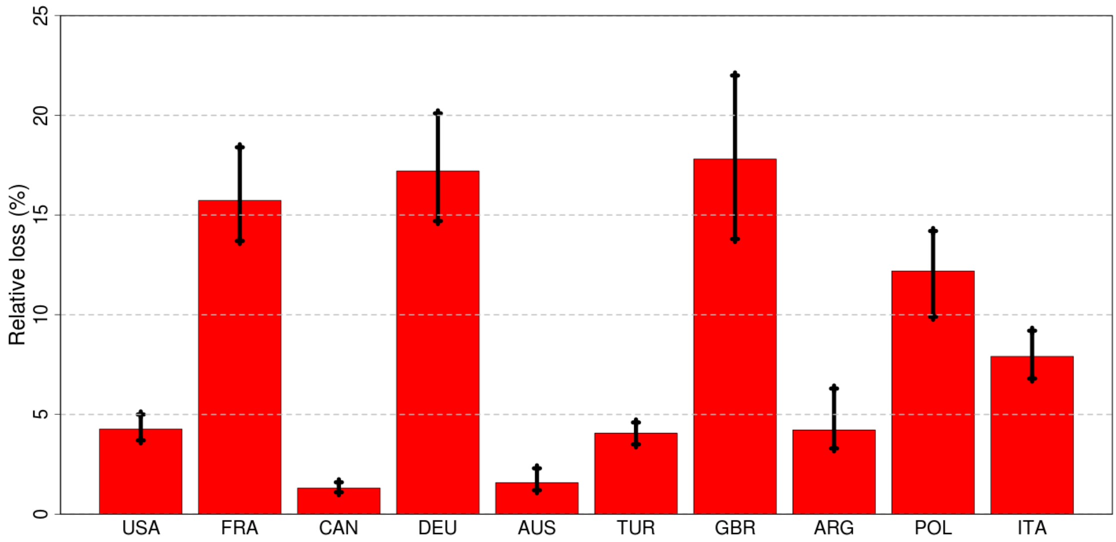
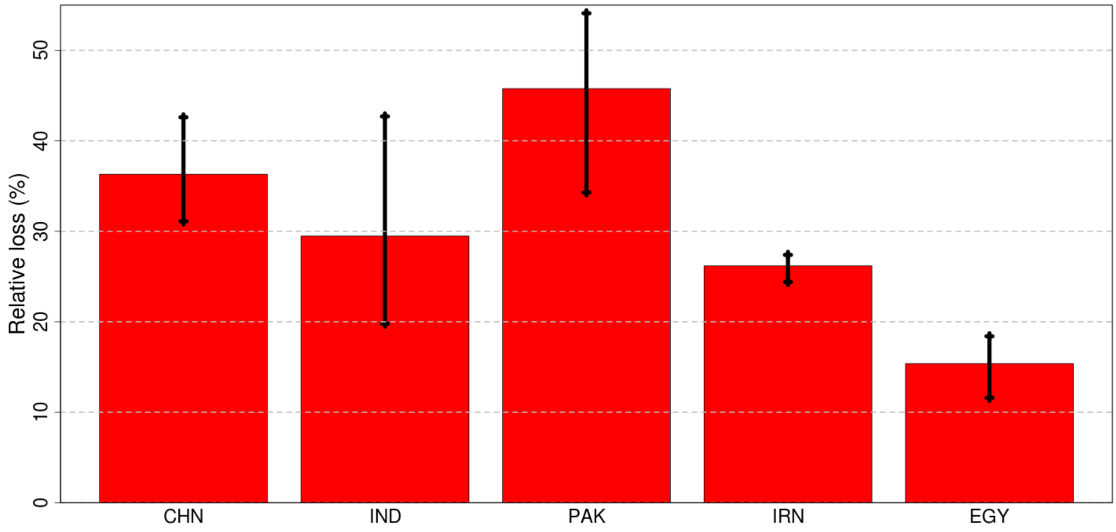


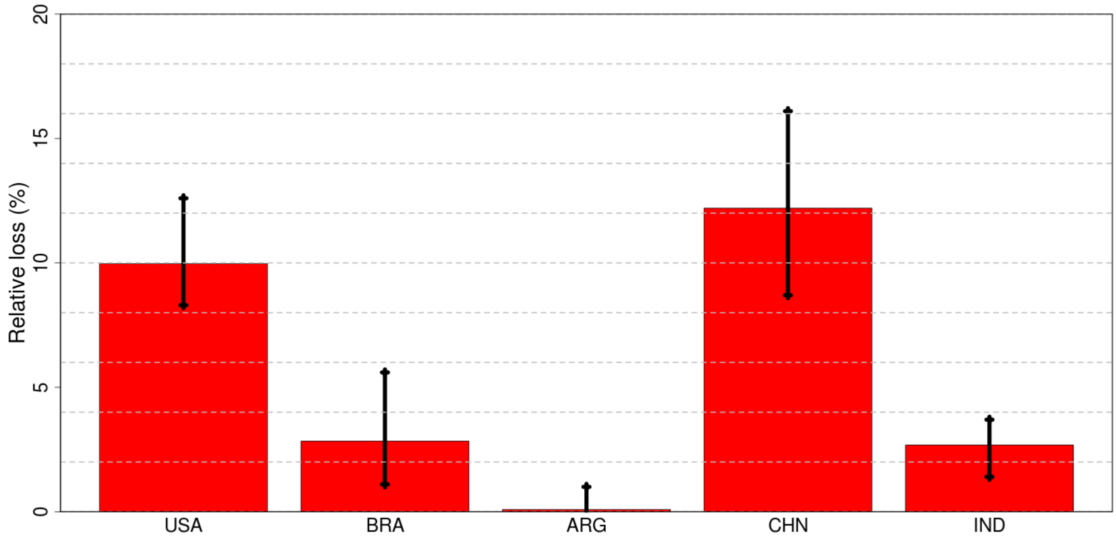
Figure S7*: Sensitivity of simulated yields to ozone parameters with marginal effects, i.e. one parameter is varied and all others are held constant at 10% of their calibrated or fixed value (tantamount to a low ozone effect). The effect of each single parameter is more pristine when the other four have little practical influence on the model. A constant temperature of 20°C, a precipitation of 6 mm per day and a photosynthetic photon flux density (PPFD) of 1,000 µmol/m^2/sec were used.*



(a) Western wheat



(b) Asian wheat



(c) Soybeans

Figure S8: *Estimated national ozone-induced yield losses when assuming globally constant high management intensity for all crops (LAImax is 5 out of 7). Panels are Western wheat **(a)**, Asian wheat **(b)** and soybeans **(c)**.*

Supplementary Tables

***Table S1**: Experimental studies used to calibrate LPJmL-O$_3$. Abbreviations of measured variables are: gs = stomatal conductance of top leaf, O$_{3up}$ = ozone uptake/flux, Asat = light-saturated photosynthesis*

Crop	Study	Location	Exp. Nr	O_3 exposure (ppb; h)	CO_2 (ppm)	Water status	Measured variables
Western wheat	Mulholland *et al.* (1997)	UK	1	84; 7	350	Unstressed	O$_{3up}$, Asat, gs, yield
			6	84; 7	550		
			7	84; 7	680		
	Farage and Long (1995)	UK	2	200; 16	350	Unstressed	O$_{3up}$, Asat, gs
			8	400; 16	350		
			9	200; 4	350		
			10	400; 4	350		
	Barnes *et al.* (1995)	UK	3	75; 6	350	Unstressed	Asat, gs
			11	75; 6	700		
	Ojanpera *et al.* (1998)	Finland	4	61; 8	350	Unstressed	Asat, yield
			12	45; 8	350		
	McKee *et al.* (1997)	UK	5	60; 4	350	Unstressed	Asat, gs
			13	60; 4	700		
	Khan and Soja (2003)	Austria	14	80; 8	375	100% of soil water holding capacity	O$_{3up}$, gs, yield
			15	80; 8	375	45%	
			16	80; 8	375	35%	
Asian wheat	Feng *et al.* (2007)	China	1	120; 8	360	Unstressed	Asat, gs, yield
	Sarkar *et al.* (2010)	India	2	70; 5	387	Unstressed	Asat, gs
			3	80; 5	387		
	Tomer *et al.* (2015)	India	4	69; 7	387	Unstressed	Asat, gs, yield
			5	75; 7	387		
	Zhu *et al.* (2011)	China	6	82; 10	387	Unstressed	Yield
			7	72; 10	387		
			8	69; 10	387		
	Biswas *et al.* (2008)	China	9	82; 7	380	Unstressed	Asat, gs, respiration
	Biswas *et al.* (2013)	China	10	72; 7	387	Unstressed	Asat, gs,
			11	72; 7	714		
	Feng *et al.* (2011)	China	12	56; 10	380	Unstressed	Asat, gs,
Soybeans	Bou Jaoudé *et al.* (2008)	Italy	1	67; 8	375	Unstressed	gs, yield
			2	67; 8	375	Stressed	
			3	67; 8	375	Unstressed	
	Booker *et al.* (2005)	USA (N Carolina)	4	82; 12	375	Unstressed	O$_{3up}$, Asat, gs, yield
			5	82; 12	698		
	Betzelberger *et al.* (2010)	USA (Illinois)	6	82; 8	375	Unstressed	Asat, yield
			7	61; 8	375		

	Betzelberger *et al.* (2012)	USA (Illinois)	8	68; 8	390	Unstressed	Asat, yield, respiration[a]
			9	81; 8	390		
			10	49; 8	390		
			11	73; 8	390		

[a] We deduced respiration indirectly from citrate concentrations, but it was not directly measured in the experiment.

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4 Consistent negative response of US crops to high temperatures

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Consistent negative response of US crops to high temperatures in observations and crop models

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High temperatures are detrimental to crop yields and could lead to global warming-driven reductions in agricultural productivity. To assess future threats, the majority of studies used process-based crop models, but their ability to represent effects of high temperature has been questioned. Here we show that an ensemble of nine crop models reproduces the observed average temperature responses of US maize, soybean and wheat yields. Each day $>30\,°C$ diminishes maize and soybean yields by up to 6% under rainfed conditions. Declines observed in irrigated areas, or simulated assuming full irrigation, are weak. This supports the hypothesis that water stress induced by high temperatures causes the decline. For wheat a negative response to high temperature is neither observed nor simulated under historical conditions, since critical temperatures are rarely exceeded during the growing season. In the future, yields are modelled to decline for all three crops at temperatures $>30\,°C$. Elevated CO_2 can only weakly reduce these yield losses, in contrast to irrigation.

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Crops grow best within specific intermediate temperature intervals. Excessive frost or heat are detrimental to physiological processes and, eventually, yield levels. Under climate change episodes of high temperature are expected to increase in frequency and duration. This could threaten regional productivity in already susceptible areas[1–4]. There are a number of statistical approaches that allow for separating effects of high temperatures on observed yields from other sources of variability that are not correlated with them over time. Rainfed maize, soybean and cotton yields in the US have been shown in statistical studies to decline non-linearly with temperatures above ~30 °C (ref. 5). Wheat in the US responds negatively to frost in fall or heat in spring; the reduction due to high temperature is lowered by increased rainfall[6]. Maize yields in Africa decline strongly with temperatures >30 °C, in particular under lack of water[7]. Senescence of irrigated wheat in India is accelerated by temperatures >34 °C (ref. 8). But these statistical models are agnostic about the underlying mechanisms, which are important to understand to help farmers better adapt to high temperatures. Process-based crop models, in contrast, provide an implementation of physiological crop growth processes. They model complex responses of crop yields to climate change, accounting for weather fluctuations on (sub-)daily time scales. In particular, they allow for varying responses in terms of the phenological state of the crop, for interactions between the atmospheric CO_2 concentration (henceforth [CO_2]), temperature, precipitation and other weather variables, and delayed effects of precipitation due to soil water storage.

High temperatures, which are defined as temperatures >30 °C within this study, affect crop yields by direct and indirect effects. High temperatures can cause water stress through depletion of soil water and increased atmospheric water demand[9–12], which leads to a closing of stomata to avoid desiccation (thereby reducing the uptake of CO_2) and also to an enhanced root growth at the expense of above-ground biomass. High temperatures can also directly damage enzymes and tissues[13–15], impair flowering[10,16], trigger oxidative stress[17], lead to precocious maturity and senescence (resulting in less time for accumulating biomass[18,19]) or lower net photosynthesis rates due to lower carbon (C) assimilation and/or higher respiration rates[20–22]. By using one site-based crop model for three corn-growing locations in the US corn belt it has been shown that the observed high-temperature effects on maize yield are largely mediated by changes in water supply and demand rather than by direct damage to the plant tissues[9]. The critical role of water availability to cope with high-temperature stress is also shown for African maize, where negative effects on yields >30 °C double under drought conditions[7].

Here we apply the statistical approach by Schlenker and Roberts[5] to simulated yields from process-based models to test their representation of observed negative high-temperature effects on a spatially aggregated level. We analyse maize, soybean and wheat, which are US staple crops occupying 62% of the 2010 harvested area in the US[23] and 33% globally[24]. To test the sensitivity to water availability, we make separate comparisons for predominantly rainfed or irrigated counties. In addition, we derive the average response to high temperature under future

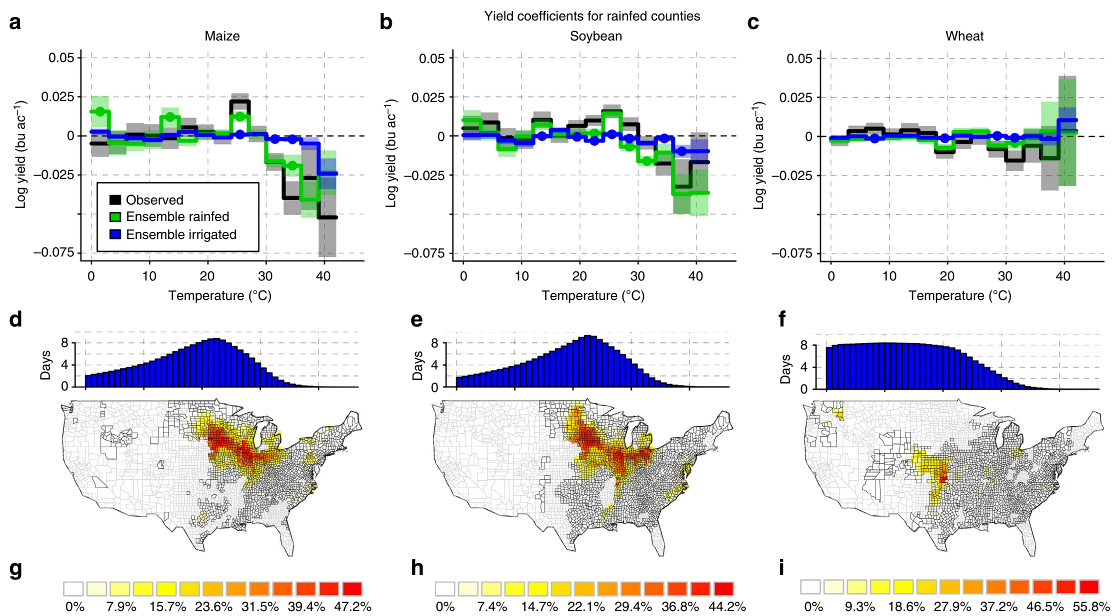

Figure 1 | Comparison of statistically estimated effects of temperatures on observed and simulated US yields in rainfed counties. Columns are maize (**a**,**d**,**g**), soybean (**b**,**e**,**h**) and wheat (**c**,**f**,**i**). **a**–**c** show regression coefficients and **d**–**f** show the histogram of times spent in individual temperature bins as the sum of times derived for each grid point across the growing seasons. **g**–**i** show rainfed counties (black outlines) with their per cent land-use share (colours) of the respective crop (for wheat only counties with predominantly winter wheat). Black lines in **a**–**c**: coefficients γ_h derived from log-transformed observed yields (Methods; equation (1)). Green/blue lines: coefficients of the ensemble median rainfed/irrigated simulated yields. Estimates are derived by a panel regression of US county data, where the considered crop is grown under predominantly (>90%) rainfed conditions. Shaded areas represent 95% confidence intervals. Simulated coefficients are marked by coloured dots if they are significantly different from the observed coefficients (confidence intervals do not overlap).

(2071–2099) climate conditions and higher levels of atmospheric CO_2 under Representative Concentration Pathway RCP8.5. While the empirical approach in ref. 5 does not account for the effects of higher [CO_2] on future yields, it is explicitly represented in process-based models. We find that the crop models of our ensemble include the most relevant mechanisms of high-temperature-induced yield loss under current climate, in particular a water-dependent temperature response in agreement with observations. Elevated CO_2 cannot be confirmed as a safeguard of yields under high temperatures, in contrast to previous assumptions. A shift of temperatures from beneficial to detrimental in a narrow temperature range can already induce large crop losses—which can reliably be assessed by current models.

Results

Models capture observed yield responses to high temperatures. The considered ensemble of nine Global Gridded Crop Models (GGCMs; eight for wheat) is able to closely reproduce the observed average response of rainfed crop yields (γ_h, Methods, equation (1)) to time spent in different temperatures from 0 to 42 °C (Fig. 1, green and black lines). The statistical model estimates the changes in yield if the crop is exposed to temperatures within individual intervals for one day. A value of $\gamma = -0.04$ as, for example, derived from the observed maize yields for the temperature interval from 33 to 36 °C means that one additional day at these temperatures would reduce the yield by $1 - \exp(-0.04) \approx 4\%$. The results are robust against the form of the statistical analysis (step function or piecewise linear, Supplementary Figs 1–3; principal component regression, Supplementary Fig. 4; Supplementary Note 1), fertilizer input (Supplementary Figs 5–7) and growing season assumptions (Supplementary Figs 8–11). In the main text, we therefore only show results for crop model-specific default representations of present-day management conditions[25] and fixed growing seasons following Schlenker and Roberts[5] (Methods).

Only 7 out of 42 coefficients significantly diverge between the regression models for observed and simulated yields (95% confidence intervals do not overlap). The confidence intervals become larger at higher temperatures, owing to less time exposed to these temperature bins. Responses for the individual models can be found in Supplementary Fig. 12; see also Supplementary Note 2. The temperature threshold of roughly 30 °C (maize and soybean peak at the 24–27 °C interval, which is one temperature bin lower than earlier estimates for maize[5]) is in close agreement with values deduced from field experiments[7,9,26,27]. In contrast to maize and soybean, wheat shows no clear temperature response pattern or decline with high temperature (Fig. 1c), neither for observed nor for simulated yields. Not all models are able to simulate winter wheat, so we excluded those which only simulate spring wheat (Methods). Given the close agreement between observed and simulated yield average responses, we use the process-based models to identify the mechanism behind the decline in yields.

Models suggest water stress as major cause of yield declines. The coefficients derived from the median of the simulated ensemble under the assumption of full irrigation (blue lines in Fig. 1) significantly diverge from the coefficients derived from simulations assuming rainfed conditions (green lines) at 7, 8 and 4 out of 14 temperature bins each for maize, soybean and wheat, respectively (cf. also the modified scaling and correlation of coefficients in Supplementary Figs 13—15; Supplementary Note 3). Full irrigation reduces the negative effect of temperatures >30 °C. Although a detrimental effect of very high temperatures >39 °C seems to occur even for irrigated maize, the

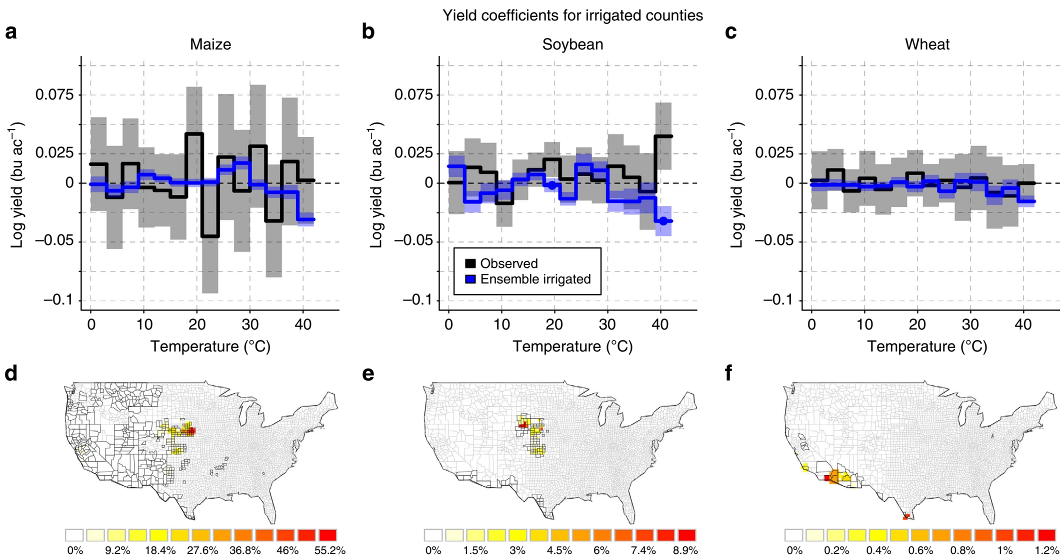

Figure 2 | Comparison of statistically estimated effects of temperatures on observed and simulated US yields in irrigated counties. Unconstrained irrigation is assumed on the irrigated areas specified by MIRCA2000 (ref. 24). Columns are maize (**a**,**d**), soybean (**b**,**e**) and wheat (**c**,**f**). **a**–**c** show regression coefficients and **d**–**f** show irrigated counties (black outlines) with their per cent land-use share (colours) of the respective crop. Counties are considered as irrigated if >75% of the crop-specific-harvested area is irrigated. Black and blue lines in **a**–**c** represent coefficients γ_h for observed and simulated yields, respectively. Shaded areas are 95% confidence intervals. Results for individual models are shown in Supplementary Fig. 33.

interpretation of this single coefficient may be misleading due to the small number of data points. In irrigated counties (Supplementary Fig. 16) neither the observations nor the simulations show a strong decline in yield coefficients at high-temperature intervals (Fig. 2; Supplementary Note 4). The confidence intervals for irrigated counties are larger, partly due to fewer observations (Methods), making the statistical model estimates noisy. The crop model ensembles for maize and soybean show a yield decline with temperatures >33 °C and 30 °C, respectively, but less pronounced than in the rainfed case. All confidence intervals in the high-temperature range are close to 0 except for 39–42 °C.

The crop model simulations assuming full irrigation on rainfed areas show a significantly higher evapotranspiration (ET; Supplementary Fig. 17) and a significantly higher biomass accumulation (Supplementary Fig. 18; Supplementary Table 3) than the rainfed runs. All models simulate shorter growing seasons with higher average temperatures for maize and soybean. For wheat the effect can be confounded by vernalization, which is delayed under higher temperatures, such that only a majority of the models shows a decrease. The average decline in length for each additional degree of average growing season temperature over the period 1980–2010 is ~7.4 days for rainfed maize, 5.6 days for soybean and 1.3 days for wheat, respectively. This decline is equal or higher under irrigated conditions in the same counties (equal for maize, but 9% and 46% higher for soybean and wheat, respectively).

Models suggest that CO_2 only limitedly attenuates yield loss. The interaction of temperature, water and [CO_2] plays an important role for future yields under global warming[17]. To assess this we apply the panel regression to simulated future yields in rainfed counties under climate change (RCP 8.5). We use an ensemble of six GGCMs (five for wheat), whose models overlap with the historical ensemble above (Methods). Four settings are analysed: rainfed conditions and fixed present-day [CO_2] levels, rainfed conditions and elevated [CO_2] (803 p.p.m. as 2071–2099 mean), full irrigation and fixed [CO_2], and full irrigation and elevated [CO_2]. Rainfed yields continue to exhibit a pronounced decline at high temperatures, even under elevated [CO_2] (Fig. 3, solid and dashed green lines). Under climate change and the associated shift of growing season temperatures into the critical range >30 °C wheat also shows a decline in yields under rainfed conditions (Fig. 3c). The signal can strongly be reduced with irrigation (blue lines) for all crops. The bottom part of each panel in Fig. 3 shows the shifts of temperature distributions over the fixed growing season into warmer ranges for the future (red solid line) when compared to the historical period (1980–2010, grey dashed line). We do not consider irrigated counties for this analysis since the historical response shows large uncertainties.

The median rainfed yields of the future model ensemble show a generally reduced temperature sensitivity caused by elevated [CO_2], also at higher temperatures for maize and wheat, evidenced by the smaller absolute coefficient values over the whole temperature range. This holds for the individual models, too (Supplementary Figs 19–21). But these reductions are not significant for any of the crops over the whole temperature range (confidence intervals overlap everywhere). In contrast, the coefficients for irrigated yields are nearly equal for fixed and elevated [CO_2] at all temperatures, for all three crops. They diverge significantly from the rainfed coefficients at 9 out of 42 coefficients, in particular in the temperature range >30 °C.

Elevated [CO_2] significantly reduces actual ET and increases biomass and yield under rainfed and irrigated conditions for all three crops (Supplementary Figs 22–25; Supplementary Table 4). For maize, however, the biomass increase with elevated [CO_2] is only marginal under irrigated conditions (4.6%) in comparison with soybean (35.2%) and wheat (19.4%). For soybean the reduction in ET at elevated [CO_2] is only marginal (1.4%) under rainfed conditions.

Discussion

We applied a statistical model to detect the temperature response of observed and simulated county yields in the US. We showed that the considered ensemble of nine process-based crop models is capable of reproducing the observed detrimental effects of high temperatures on rainfed maize and soybean crops. For wheat neither observations nor simulations show a decline in the historical period. The close agreement between rainfed simulations and observations and a strongly reduced yield decline with ample water supply in the models allows us to

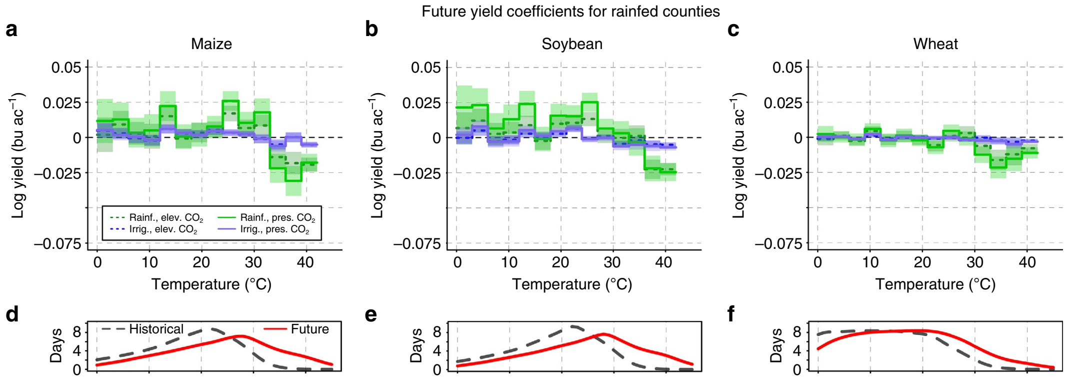

Figure 3 | Simulated yield responses to temperature under future climate change in rainfed counties. Columns are maize (**a**,**d**), soybean (**b**,**e**) and wheat (**c**,**f**). **a**–**c** show regression coefficients and **d**–**f** display temperature histograms for the historic (dashed grey) and future (solid red) periods; future climate is evaluated over 2071–2099 based on RCP8.5. Green tone lines in **a**–**c** are ensemble yield responses to temperature under rainfed conditions. Blue tone lines are ensemble yield responses under irrigation. Solid lines are derived with fixed present-day [CO_2], while dotted lines include elevated [CO_2] according to RCP8.5. Shaded areas are 95% confidence intervals. Rainfed counties are defined in Fig. 1.

conclude that irrigation lowers the temperature sensitivity of all three crops. In the future, the models suggest a negative response of maize, soybean and wheat to high temperatures even under elevated [CO_2]. A future shift of temperatures from beneficial to detrimental may reduce crop yields substantially even without considering the effect of extremely high temperatures.

Negative effects of high temperature on wheat would be expected at temperatures >30 °C (ref. 26). Under historical conditions wheat was usually harvested before high-temperature stress occurred, or the stress occurred during non-sensitive phenological stages. The occurrence of temperatures >30 °C per growing season is, on average, higher for maize (10.8 days) and soybean (13.1 days) compared with wheat (6.0 days). Field trial data in Kansas[6] has shown sensitivity of wheat to temperatures above 34 °C in spring, which we do not observe for the larger geographic coverage and given the rare occurrence of such spring heat events in the past.

The close agreement of high-temperature responses of observed and simulated yields allows for an investigation of the underlying mechanism of the yield decline. In particular, the threshold response >30 °C, which is not natively implemented in the models, is a prerequisite for this investigation. The dampening effect of irrigation on the temperature response of yield supports the hypothesis that temperature-induced water stress is the main driver of the observed yield decline at temperatures >30 °C, in line with the study by Lobell *et al.*[9] Atmospheric water demand increases with temperature as an immediate effect. In addition, water supply from soil to plant gradually decreases due to depletion of soil water stocks from sustained high ET. Both factors can lead to water stress for crops, where the stomata gradually close to prevent water loss and therefore preclude the diffusion of CO_2 into the cells. This leads to a reduced gross photosynthesis rate. All GGCMs considered here represent both the immediate (stomatal closure) and progressive (soil water depletion) effects of temperature (model characteristics in Supplementary Table 1). In addition, crops respond to water stress by enhanced root growth at the expense of above-ground biomass and yield; this effect is included in eight of the nine models (Supplementary Table 1). The critical role of water supply at high temperature is further supported by the yield response curves for observed yields from predominantly irrigated counties, where no clear temperature response is visible. Yet this yield response in irrigated counties is rather noisy due to few observations (Methods). But our conclusions mainly rely on the (counterfactual) irrigated yield response in rainfed counties, where a larger panel allows for robust assessments. Troy *et al.*[28] have recently shown that irrigation attenuates the yield impacts of several climate-extreme indices, which is in accordance with our findings. Thus reduced gross photosynthesis rate, triggered by reduced CO_2 inflow under water stress, constitutes a major pathway for yield decline under high-temperature conditions without sufficient water supply (first point from the effects listed in the introduction).

Yet the existence of temperature-induced water stress does not necessarily preclude other negative effects of high temperatures (other points from the list above). The first three of the alternative explanations (direct damage to enzymes and tissue, impaired flowering and oxidative stress) are not represented in the considered crop model ensemble (except impaired flowering in one model, PEGASUS). That the ensemble is nevertheless able to reproduce the observed decline in yields at temperature levels of 30–36 °C suggests that these three effects are not the main causes of the observed decline in yields in this temperature range at this spatial coverage. Direct damage to enzymes, tissues or reproductive organs is only expected at higher-temperature levels (35–37 °C for maize and 35–39 °C for soybean; refs 26,27) than the thresholds identified here. The actual leaf temperature could deviate from the surrounding air temperature, since water scarcity precludes a transpirational cooling of the leaves. Yet, none of the considered models explicitly accounts for leaf temperature differences to ambient air. Furthermore, there is evidence that irrigation does not only reduce the perceived temperature for the plant, but also the actual temperature over large regions[29–31]. This effect is not considered in the crop models. But given the agreement between observations and simulations, a direct damage seems to be of minor relevance for the general shape of the temperature response at the range considered here. Increasing oxidative stress can arise from higher levels of photorespiration or higher uptake rates of ozone (O_3), whose concentrations tend to increase with temperature[32]. A potential increase in photorespiration is expected to be less pronounced in C_4 plants like maize[13,17,22], which is not supported by the observational data showing a particularly pronounced decline in maize yields. For O_3, irrigation could even increase its damaging effects, since more available water allows the stomata to open wider, which would let more O_3 in ref. 33. Thus, the first three alternative pathways do likely not explain the observed yield reduction under rainfed conditions and its alleviation under irrigation.

In contrast, the crop models do simulate shorter growing seasons with increasing temperature(Supplementary Table 5). The phenological development of crops is mainly controlled by temperature, such that (non-adapted) crop plants would have less time for gaining biomass and yield if the growing season shortens. This could explain yield declines with high temperature. But in the model ensemble the growing season lengths shorten equally or even more for irrigated yields than rainfed yields. So a shorter maturity time does not explain why there is no reduction in yields for irrigated conditions. In addition, observations show that maturity may even be delayed, instead of advanced, by high temperatures[9,34].

Seven of nine models include a direct effect of temperature on maintenance respiration (Supplementary Table 1), and the other two have a lower radiation use efficiency under high-temperature stress. Net biomass gain is the difference between gross photosynthesis and plant respiration, such that an increased respiration can lead to lower biomass and yield. Respiration data are not available from the model ensemble considered, but the relative share of respiration to assimilation is expected to increase with high temperature[22] and water stress[15]. An evaluation of the 2003 European heat wave, however, found a decreasing respiration under heat and drought conditions[21]. Respiration equations in the models are influenced by temperature only, not by water supply. Therefore increased respiration under high-temperature stress does not explain why there is no yield decline under irrigation, in particular since models have no cooling effect of transpiration on perceived temperature. Together with the ambiguous response of respiration to high temperature or drought stress, we suggest that increased respiration is not a primary reason for the yield decline under high temperatures within the range analysed here.

The statistical approach is sensitive to yield losses induced by extremely high temperatures, despite their low relative abundance in the data set (Supplementary Fig. 26; Supplementary Note 5). At the same time, the direct damage to enzymes, tissues or reproductive organs expected in these temperature ranges is not represented in the crop models (see above). Thus, the agreement between observations and simulations indicates that damage directly induced by extremely high temperatures is of minor relevance in the historical sample on the large spatial scale of our study. Damages in the observed yields could be limited if temperatures occurred in noncritical periods of the growing season. But in the considered sample extreme temperatures mainly occurred in the middle and last phase of the growing season, in which anthesis and grain filling mostly occur (Supplementary Fig. 27). Both these processes are known to be critically sensitive to high temperatures[8,10,20,22,35–37]. In addition, a sensitivity test regarding the timing of the exposure and the definition of the growing season has not revealed a significant difference in the associated responses to extreme temperatures[5]. Evaporative cooling may have reduced leaf temperatures to lower values than air temperatures, which are used as predictor in the regression model. The latter aspect is not represented in the crop models and requires further work to quantify the role of evaporative cooling, as a protection mechanism[38,39]. In addition, harvests may have been adjusted to avoid exposure to extremely high temperatures, an effect not represented in the exposure times used in our analysis. Yet, given the abundant total number of such extremely high temperatures in our data set (41,580 days $>36\,°C$ for maize, 70,934 for soybean and 34,200 for wheat), we argue that the latter explanation is less relevant. The agreement between the observed and simulated temperature sensitivities found for the historical sample does not imply that models capture all processes relevant under future climate change, where direct temperature-induced damages may become more relevant. However, based on the regression coefficients derived from the historical observations and temperature shifts projected for the end of the century by HadGEM2-ES under RCP8.5, increasing exposure to temperatures in the range from 30 °C to 36 °C alone implies yield losses of 49% for maize, 40% for soybean and 22% for wheat (Table 1). Our analysis suggests that crop models reliably simulate temperature effects in this range. A further test of the reliability of future projections of yield losses could be achieved by assessing regions that are already warmer today, or of field experiments where temperatures are artificially increased[40,41].

Assuming that the crop models are able to capture the relevant mechanisms that lower yields at high temperatures, as discussed above, we continue to investigate the simulated future interactions between high temperature, water supply and CO_2 concentrations. We only consider rainfed counties (maps in Fig. 1), since the estimates of the statistical model in irrigated counties (Fig. 2) are too noisy to base any extrapolation on them. An elevated concentration of CO_2 is reported as a yield-increasing factor for most plants[12,32]. It tends to increase crop water-use efficiency (gain of carbon per unit of water lost) and maintain higher levels of soil moisture. Observations have confirmed that CO_2 fertilization is usually more efficient under drought conditions, even for C_4 plants such as maize[17,42]. But the only insignificant differences in high-temperature response of yields with elevated $[CO_2]$ suggest that elevated $[CO_2]$ has a limited potential to buffer against detrimental effects of temperature-induced water stress on crop yields. These findings do not contradict beneficial effects of CO_2 on yield, in particular when integrating over the growing season (Supplementary Fig. 25). But they suggest that episodic temperature-induced water stress cannot be attenuated effectively with higher $[CO_2]$ alone. In particular for soybean elevated $[CO_2]$ leads to more biomass (larger leaf area), which in turn increases transpiration needs (Supplementary Fig. 23). Thus, the amount of water required by soybean under elevated $[CO_2]$ is similar to that under fixed $[CO_2]$, despite higher water-use efficiency. As a consequence the plant responds in a similar way to the water stress triggered by elevated temperature. Thus, a strong biomass increase under elevated $[CO_2]$ prevents an ameliorating effect of $[CO_2]$ under episodic temperature-induced water stress (similar conclusions are derived in refs 9,17,43,44). For wheat (C_3) and maize (C_4) the biomass increase under elevated $[CO_2]$ is smaller (Supplementary Figs 22 and 24). Therefore, the temperature-induced water stress can better be attenuated with higher $[CO_2]$ in these two crops when compared with soybean, but still not significantly. These hypotheses are based on model results in rainfed counties only, where a robust response to temperature is visible for simulated rainfed and irrigated yields (Fig. 1), and could guide further experiments on the role of CO_2 under high-temperature stress.

Estimated yield responses under high levels of global warming should not be interpreted as predictions, since the GGCM simulations do not commonly account for potential adaptation options. The implementation of management and thus adaptation options differs between models. For example, fertilizer application rates were held constant (PEGASUS, pDSSAT and pAPSIM) or adjusted flexibly according to nitrogen stress (EPIC-IIASA, EPIC-BOKU and GEPIC). The choice of cultivars was only allowed to change trough time in PEGASUS, LPJ-GUESS and limitedly in GEPIC. Thus, the ensemble response to temperature exposure represents the average response across a range of different management assumptions. Individual farmer's options to adapt to more frequent temperature stress could dampen negative yield responses—though the extent may be limited[5,45].

The effects of CO_2 on yield formation are taken from the individual models' best estimate, which have partly been calibrated against experiments to capture yield responses to CO_2 (ref. 46). There is a discussion that crop models may overestimate yield response to elevated levels of CO_2 (refs 42,47). Furthermore, an adequate sensitivity of the models to temperature or water supply does not imply any conclusions on the adequacy of the CO_2 effect in models. Caution needs to be exercised also when extrapolating historical temperature

Table 1 | Contribution to yield changes by different temperature ranges.

Crop	Time	Yield change factors				Future yield loss below 36 °C
		Below 30 °C	30–36 °C	Above 36 °C	Total	
Maize	Historical	1.80	0.73	0.96	1.27	49%
	Future	1.62	0.41	0.47	0.31	
Soybean	Historical	2.84	0.88	0.95	2.37	40%
	Future	2.12	0.71	0.59	0.89	
Wheat	Historical	0.93	0.91	0.99	0.84	22%
	Future	0.85	0.78	0.94	0.62	

Numbers are yield change factors for different temperature ranges that modify the base yield resulting from intercept, precipitation, county-fixed effects and time trends. The total column indicates the product of all temperature exposures $>0\,°C$ on yield. The last column indicates yield loss expected from a shift of temperature exposures only within the 0–36 °C range (calculated with equation 2).

responses into the future, as temperature effects that are of minor relevance in the past may become more important in the future, in particular in temperature ranges not observed in the historical data set. Direct crop damages from extremely high temperatures (for example, 40 °C) are usually not represented in current crop models and would have to be improved before assessing crop responses to these extremes in the future[48]. But already the shift towards higher temperatures from beneficial to detrimental (histograms in Fig. 3), without considering extreme temperatures, poses a strong challenge for rainfed crop production (Table 1). An increase of irrigated areas or irrigation efficiency to overcome (parts of) the negative consequences would be effective. Yet potential constraints of water availability have to be accounted for refs 49–51.

Some of the models in our historical and future ensembles belong to model families with a shared history of development. Specifically, the three EPIC-based models (EPIC-Boku, EPIC-IIASA and GEPIC) share an identical model core, but have distinct assumptions on input and crop-specific parameters, and the two LPJ-type models (LPJ-GUESS and LPJmL) share the same photosynthesis approach, but diverge, for example, in allocation or crop-specific assumptions. Yet a shared model history does not prescribe a similar response to environmental conditions. This is exemplified by the different responses of models even of the same families (Supplementary Figs 8–10), which is comparable to differences between models of distinct families. As a consequence we assume the confidence intervals and model ensembles to be unbiased with respect to model families.

Our study provides insight into high-temperature-induced mechanisms of yield losses at an aggregate scale and thus constitutes a complement to field-based or experimental studies. The latter allow for a direct control of temperature and confounding variables, but are necessarily restricted to few locations and have until now only sparse coverage of the whole US[40,41,52]. Therefore experimental bottom-up and top-down regression approaches are both necessary to elucidate crop responses under climate change. The applied statistical approach allows extracting average yield responses to exposure to different temperature bins across a large spatial area with varying small-scale management conditions. As such it is particularly suitable for the evaluation of GGCMs rather designed to reproduce yields responses on large scale than to resolve fine-scale variations in management. It adds to well-established knowledge of yield responses to temperature that is derived from field and chamber experiments. The application of GGCMs may help us to explore adaptation options on large scales.

The crop models used here do not represent all potentially detrimental effects of high temperature. Short-term changes in management, such as fertilizer input, or diseases and pests also influence observed yield fluctuations[53], but are often not well documented and also not always represented in the models. But the simulations show a water-dependent temperature response that is in agreement with the observations. Therefore, we infer that the crop models include the most relevant mechanisms under current climate. Though extreme temperatures will become more important under climate change, and crop models will have to capture the associated effects[48] , already the shift in the exposure times to temperatures in the range from 30 to 36 °C can induce large crop losses—which can reliably be assessed by current models. Despite the clear ensemble response, there are several cases where the combined temperature water effects are either under- or overestimated, and this behaviour should be investigated further in the process-based models. The accurate simulation of yield response to temperature does not necessarily imply an accurate reproduction of observed yield time series, since other factors like management could mask them. We suggest further field experiments to assess our model-based hypothesis of a limited effect of elevated [CO_2] under water stress induced by high temperatures. In addition, models with an explicit representation of leaf temperature could help to deepen our understanding of the processes involved in yield decline under high temperatures and further improve crop projections under climate change.

Methods

Climate data. Historical: we employed daily temperature (maximum and minimum) and precipitation data for the statistical model, and further weather variables for the yield simulations by the GGCMs, from the AgMERRA climate data set[54], covering the years 1980–2010. The weather data were spatially aggregated to 0.5° for the crop simulations[25]. We used the identical data set for the statistical analysis. Its spatial resolution is one order of magnitude coarser than in the original empirical study[5], which could result in less temperature extremes due to aggregation effects. But the slight deviation between the temperature distributions of the two data sets (Supplementary Fig. 29,30; Supplementary Note 6) only has a minor effect on the estimated coefficients (Supplementary Fig. 31). In addition, predicted yields from the regression model based on the AgMERRA data are in close agreement with the observed yields in terms of mean growing season temperatures (Supplementary Fig. 32). Future: all future model results (statistical and process-based) are forced by bias-corrected[55] climate projections from the HadGEM2 climate model under the RCP8.5 scenario at 0.5° spatial resolution. We applied only one climate model, instead of an ensemble, since we study relative temperature responses rather than absolute yield levels.

Yield data. Historical observed US county yields from 1980 to 2010 (to 2008 for wheat) were downloaded from the USDA Quick Stats tool[23]. Historical yield simulations were calculated under the default and harmnoN harmonization scenarios (differing in fertilizer input, growing season definition and irrigation choices, cf. ref. 25) by nine different crop models: EPIC-Boku, EPIC-IIASA (both, ref. 56), GEPIC[57], LPJ-GUESS[58], LPJmL[59], ORCHIDEE-crop[60], pAPSIM[61], pDSSAT[62] and PEGASUS[63]. All GGCMs are forced by the same climate input[54], which is also used to calculate the time of the growing season that is spent within the different temperature bins. Historical model yields were generated within the GGCM Intercomparison project[25] of the Agricultural Modelling Intercomparison and Improvement Project (AgMIP[64]). Future yield simulations (years 2071–2099) were taken from the Inter-Sectoral Impacts Model Intercomparison Project (ISI-MIP[65]) Fast-Track data archive, once with CO_2 fixed at present-day levels (364–380 p.p.m. for all except pDSSAT which uses 330 p.p.m.) and once with elevated CO_2 (803 p.p.m. as 2071–2099 average). Yields from six models were available: EPIC-Boku, GEPIC, LPJ-GUESS, LPJmL, pDSSAT and PEGASUS. Note that model results for historical and future simulations were submitted at different times (future: 2011, historical: 2014 onwards); therefore, a direct comparison between the two responses is possibly biased due to differences in model versions. PEGASUS is excluded from both wheat ensembles, since it only simulates spring wheat. The crop models have not been calibrated against the observed temperature response used for validation here.

Derivation of times spent in different temperature bins. In analogy to ref. 5, we calculated the days spent in each 1° temperature bin during a fixed growing season (from March 01 to August 31 for both maize and soybean, and October 15 to July 15 for wheat) for each grid cell, using a sinus interpolation between daily minimum and maximum temperature. We then aggregated this data to county level with the MIRCA2000 land-use pattern[24], weighting by irrigated and rainfed shares, and considered only aggregated 3-K temperature bins as in ref. 5. In addition to the fixed growing season, the calculation was repeated for the model-specific growing seasons. For the future period from 2071 to 2099 the times spent in individual temperature bins were derived analogously, based on the bias-corrected climate projections.

Regression model. We pool the US county yields for each crop and irrigation setting to achieve a higher frequency of the rare high-temperature events in our data set (also pursued in ref. 28). A panel regression, implemented in R and following the procedure in ref. 5, was fitted separately to observed and simulated crop yields for all US counties, individually for rainfed and irrigated counties. A county was classified as rainfed or irrigated if its crop-specific area share was at least 90% rainfed or 75% irrigated, respectively. Mixed counties (rainfed share between 25 and 90%) were excluded. The following equation was applied for fitting:

$$\log Y_{it} = \alpha_0 + \sum_{h=0,3,6,\ldots}^{39} \gamma_h [\theta_{it}(h+3) - \theta_{it}(h)] + \mathbf{z}_{it}\delta + c_i + \varepsilon_{it} \qquad (1)$$

where Y is yield, log the natural logarithm, i the county and t the year. $\theta_{it}(h)$ is the cumulative distribution function of days during the growing season spent at temperature h, and the γ_h represent the estimated scaling coefficients shown in Figs 1–3. In addition, the model adjusts for a common intercept to all counties α_0 and county-specific fixed effects c_i. Variations in precipitation (linear and quadratic) and state-specific time trends (linear and quadratic) to capture technological change are subsumed in $\mathbf{z}_{it}$ with the fitted scaling factors δ. The residual error is described by ε_{it}; these error terms are allowed to correlate spatially as in ref. 5, estimated with the non-parametric method proposed by ref. 66, and applying a cutoff of 3° spatial distance. All temperatures $>39\,°C$ were subsumed into the same bin for 39–42 °C (mean value before pooling is 40 °C for all three crops), while the effect of temperatures $<0\,°C$ is captured by the fitted intercept. The total number of rows in the panels for historical observed rainfed maize, soybean and wheat are 42,648, 41,920 and 38,845, respectively, and 2,277, 719, and 149 county-year entries for irrigated counties. The total number of parameters to be fitted is ~ 80 for rainfed counties and ~ 25 for irrigated counties (depending on the number of states in the panel).

Contribution of temperature shifts to yield losses. We split the temperature distribution into three parts: $<30\,°C$ (no stress), 30–36 °C (medium high temperature) and $>36\,°C$ (extreme high temperature; consistent with previous thresholds[8,35–37,67,68]). We calculate the relative contribution to yield for each of these parts by multiplying the coefficients estimated from observed yields with the historical or future exposure time for each 3 °C bin. This results in change factors that modify the base yield resulting from intercept, precipitation, county-fixed effects and time trends. Yield loss by exposure shifts up to 36 °C is then calculated with the ratio of these factors (equation 2).

$$\text{loss} = 1 - \frac{e^{\sum_{h=0,3,6,\ldots}^{33} \gamma_h \left[\theta_{\text{avg}}^{\text{fut}}(h+3) - \theta_{\text{avg}}^{\text{fut}}(h)\right]}}{e^{\sum_{h=0,3,6,\ldots}^{33} \gamma_h \left[\theta_{\text{avg}}^{\text{hist}}(h+3) - \theta_{\text{avg}}^{\text{hist}}(h)\right]}} \tag{2}$$

Code availability. All codes (R scripts) necessary to reproduce our results are available from the corresponding author on request.

Data availability. All data supporting the findings of this study are either public data sets, are available within the article and its Supplementary information files or are available from the corresponding author upon request.

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Author contributions

B.S. and K.F. designed and performed the analysis and wrote the paper. W.S. originally designed the regression approach of yields to temperature exposure. All other authors contributed model results, helped to analyse data and commented on the manuscript.

Additional information

Supplementary Information accompanies this paper at http://www.nature.com/naturecommunications

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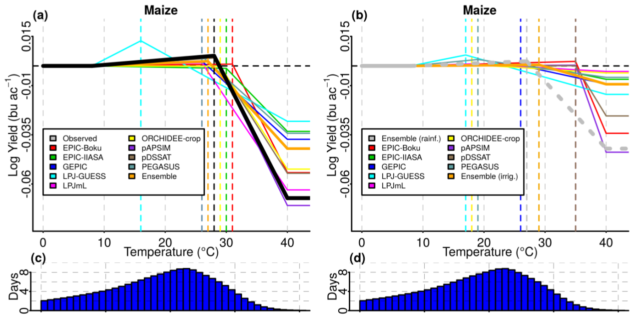
4.2 Supplementary Information

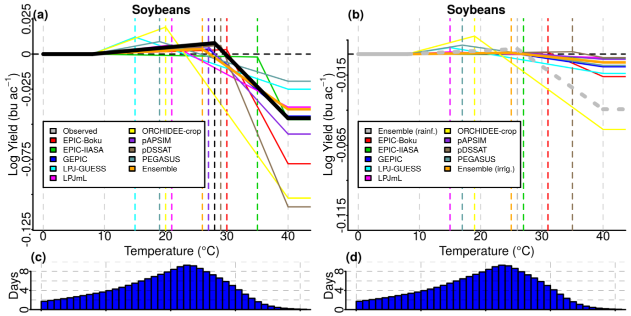
The supplementary information is printed in scaled form since its original version is also available with the online version of the article.

Supplementary Information: “Consistent negative response of US crops to high temperatures in observations and crop models”

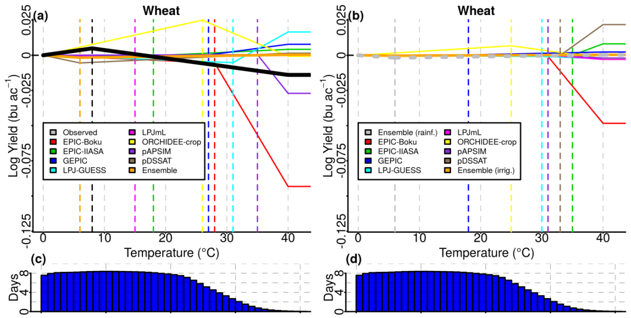
Supplementary Figures



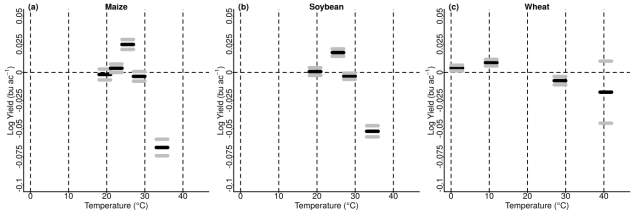
Supplementary Figure 1: Regression of US maize according to the “piecewise linear” approach in rainfed counties. Panels (**a,b**) show regression coefficients and panels **(c,d)** display the temperature exposure during an average, fixed growing season. Yields in panel (**a**) are rainfed while yields in panel (**b**) are irrigated. The rainfed ensemble line is drawn for comparison also in panel **(b)** (grey dashed line). The pattern of yield response to temperature exposure is clearly visible for the rainfed yields: a significantly positive response to intermediate, but a strong negative response to high temperatures, both in observed and simulated yields (panel **a**). For simulated irrigated yields, in contrast, a significant inflection point from high temperature damage is missing (six models + ensemble; panel **b**) or occurs only at higher temperatures and less pronounced (EPIC-Boku, pAPSIM and pDSSAT).



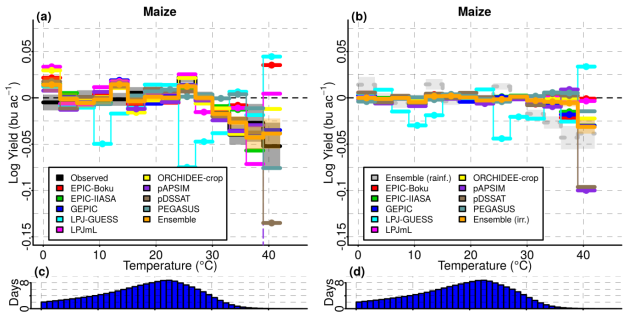
Supplementary Figure 2: Regression coefficients of US soybean according to the “piecewise linear” approach in rainfed counties. Panels and colors are as in Supplementary Figure 1.



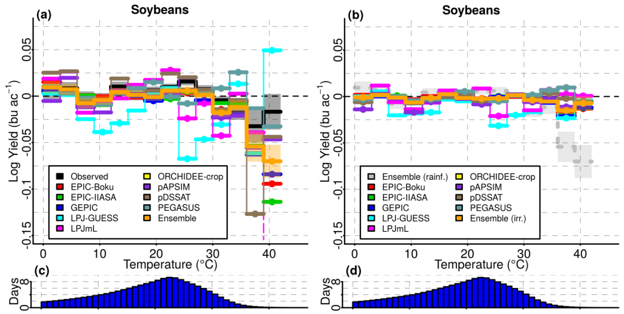
Supplementary Figure 3: Regression of US wheat according to the “piecewise linear” approach in rainfed counties. Panels and colors are as in Supplementary Figure 1.



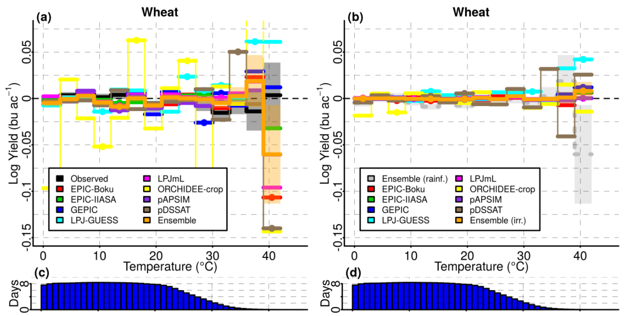
Supplementary Figure 4: Regression analysis for principal temperature components only. Rainfed observed maize (panel **a**), soybean (panel **b**) and wheat (panel **c**) show the same responses as with the full regression frame. Black lines show coefficients and grey lines show 95%-confidence intervals.



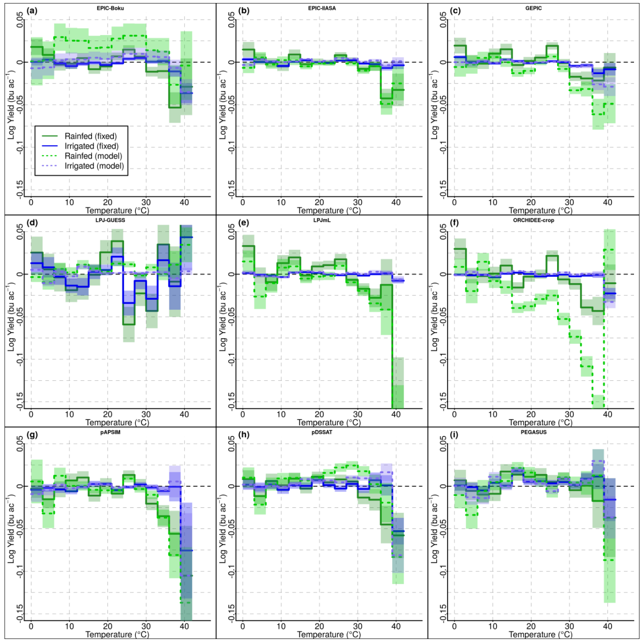
Supplementary Figure 5: Regression coefficients for **(a)** rainfed and **(b)** irrigated simulated maize. The black curve in panel **(a)** shows the observed yield response, while the grey curve in panel **(b)** shows the *simulated rainfed* ensemble response for comparison. The simulation runs were performed under the 'harmnoN' scenario (see text) in rainfed counties. Panels **(c,d)** show temperature exposures during an average, fixed growing season. Colored lines indicate different models. More details about the two simulation scenarios can be found in ref.[1]. Results are shown for the 'fixed' growing season, but are not qualitatively different for the model-specific growing seasons (data not shown).



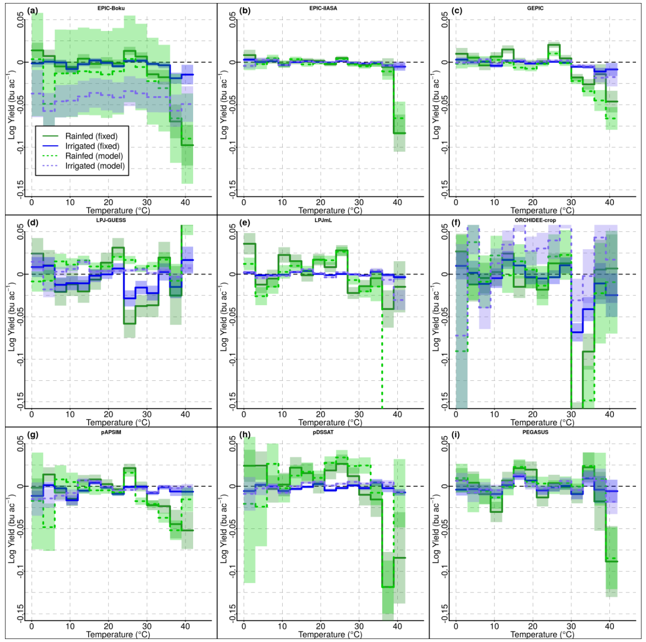
Supplementary Figure 6: Regression coefficients for **(a)** rainfed and **(b)** irrigated simulated soybean under the 'harmnoN' scenario. Panels **(c,d)** show temperature exposures during an average, fixed growing season. Colors are as in Supplementary Figure 5.



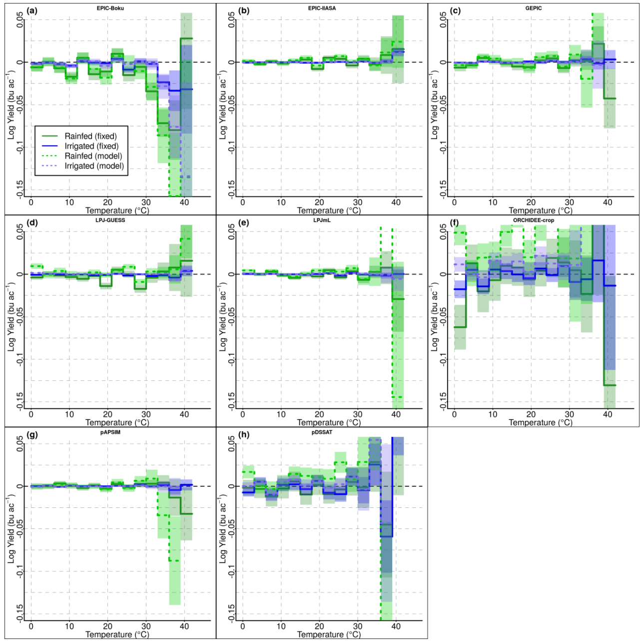
Supplementary Figure 7: Regression coefficients for **(a)** rainfed and **(b)** irrigated simulated wheat under the 'harmnoN' scenario. Panels **(c,d)** show temperature exposures during an average, fixed growing season. Colors are as in Supplementary Figure 5.



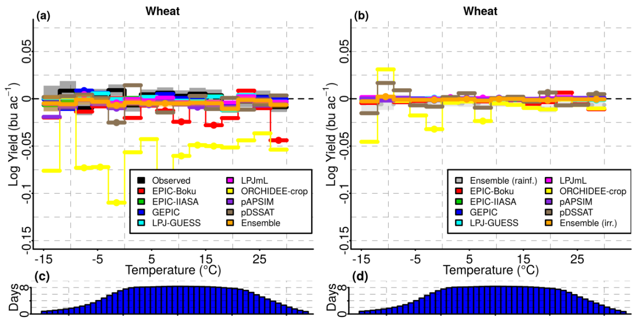
Supplementary Figure 8: Regression coefficients for US maize from the nine individual crop models used in our ensemble. For each model four setups are analyzed: rainfed with fixed (March 01 – August 31) growing season (solid green) or model-calculated growing season (dashed green), and irrigated with fixed (solid blue) or model dates (dashed blue). Shaded areas are 95% confidence intervals. A note on LPJ-GUESS: the low average yield amount simulated by LPJ-GUESS (in the considered region) inherently increases yield variability; this may lead to a reduced signal-to-noise ratio, which is the likely reason behind the unique temperature response of this model.



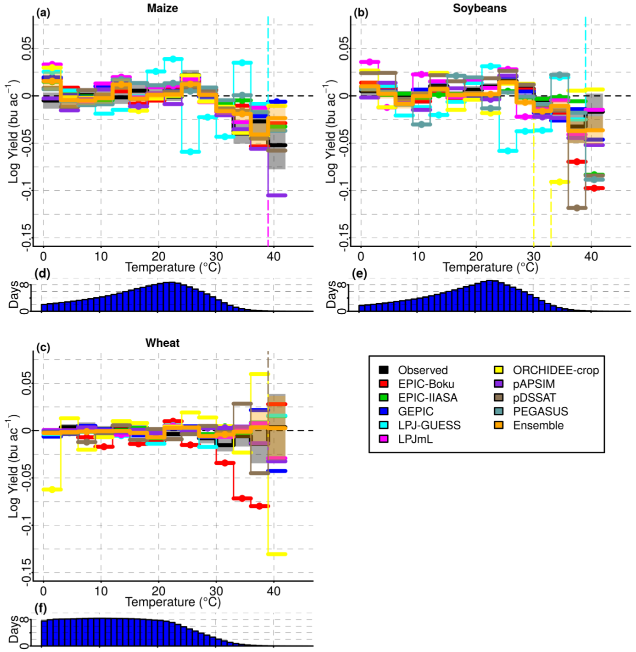
Supplementary Figure 9: Regression coefficients for US soybean from the nine individual crop models used in our ensemble. Colors are as in Supplementary Figure 8. For LPJ-GUESS and ORCHIDEE-crop the same arguments apply as for maize.



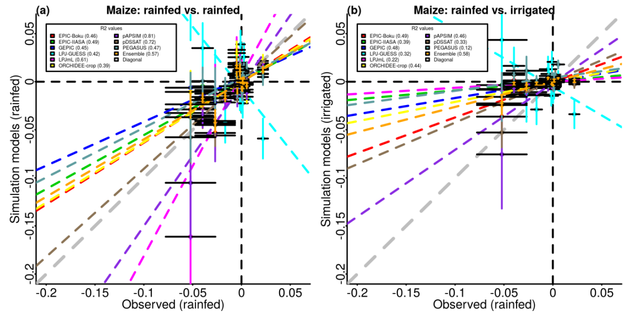
Supplementary Figure 10: Regression coefficients for US wheat from the nine individual crop models used in our ensemble. Colors are as in Supplementary Figure 8.



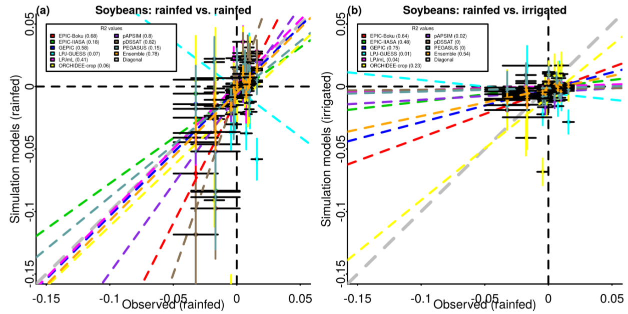
Supplementary Figure 11: Wheat response to temperature, with a broader temperature range down to -15°C, in rainfed counties. Panels **(a,b)** show yield responses to different temperature bins with **(a)** rainfed or **(b)** irrigated simulations. Panels **(c,d)** show temperature exposures during an average, fixed growing season. Colored lines represent individual models. The grey dashed line in panel **(b)** is the simulated rainfed ensemble response for comparison (orange line in panel **a**).



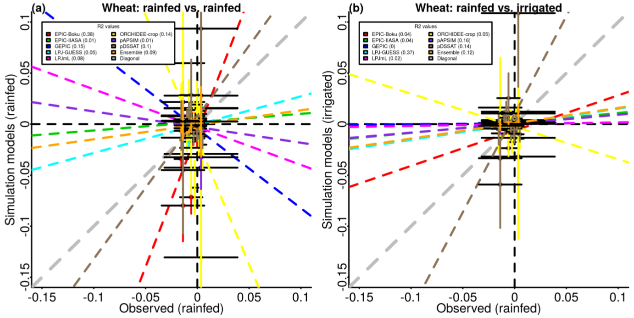
Supplementary Figure 12: Comparison of simulated to observed effects of high temperatures on rainfed yields in rainfed counties. Panels **(a-c)** show coefficients for **(a)** maize, **(b)** soybean and **(c)** wheat. Panels **(d-f)** show the mean temperature exposure over the analyzed area, averaged over all years. Black lines in panels **(a-c)** are coefficients (γ_h) for log observed yield if the crop is exposed for one day to a particular 3°C temperature interval. Colored lines are coefficients for the simulated yields (orange = ensemble median). Estimates are derived by a panel regression (equation 1) of US county data where the considered crop is grown under predominantly (> 90%) rainfed conditions. Grey and orange shaded areas represent 95% confidence intervals. Coefficients for observed yields significantly differing from 0 are marked with a black dot. Simulated coefficients are marked by colored dots if they are significantly different from the observed coefficients (confidence intervals do not overlap). The analysis is based on the assumption of a fixed growing season following ref. [2].



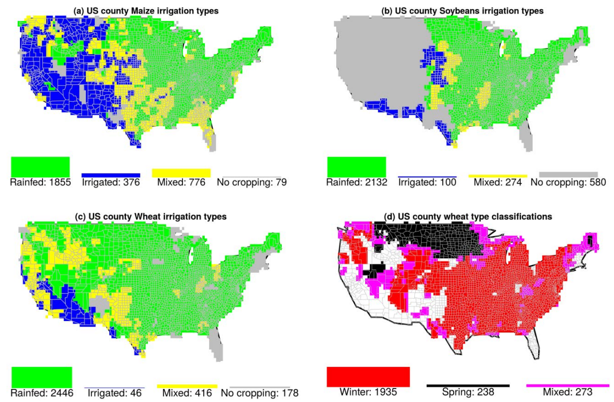
Supplementary Figure 13: Correlation plots of temperature coefficients for simulated rainfed (panel **a**) and irrigated (panel **b**) vs. observed rainfed maize in the US, all for rainfed counties. On the x-axis the coefficients for the regression with rainfed observed yields are shown, while on the two y-axes the coefficients of the different crop models are displayed. In panel **(a)** both observed and simulated yields are rainfed, while in panel **(b)** the observed yields are still rainfed, but the simulated ones are irrigated. Different colors denote different models, and numbers in brackets in the legend indicate the R^2 for each model-to-observed linear correlation of coefficients. The lines around points are 95% confidence intervals. Gray dashed lines are 1:1 lines for comparison.



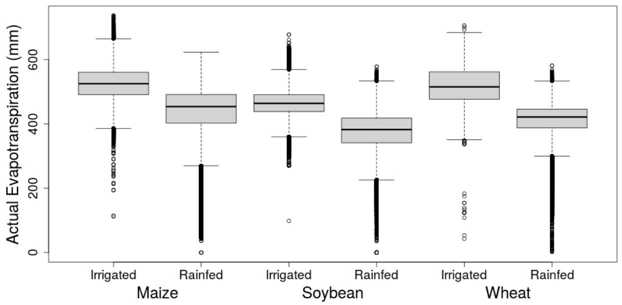
Supplementary Figure S14: Correlation plots of temperature coefficients for simulated rainfed (panel **a**) and irrigated (panel **b**) vs. observed rainfed soybean in US rainfed counties. Colors are as in Supplementary Figure 13.



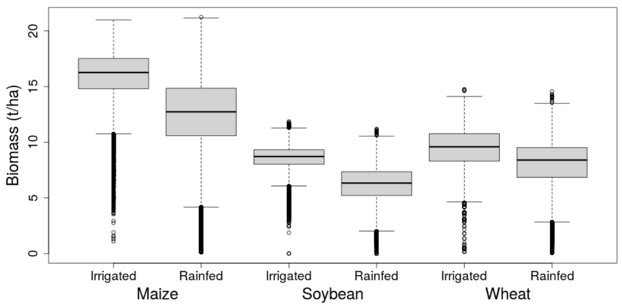
Supplementary Figure 15: Correlation plots of temperature coefficients for simulated rainfed (panel **a**) and irrigated (panel **b**) vs. observed rainfed wheat in US rainfed counties. Colors are as in Supplementary Figure 13. There is no pattern in either of the two water supply scenarios, indicating that temperature-induced water stress does not play a major role for historical wheat yields. Negative slopes can occur spuriously from a clustering of the coefficients around 0 with large confidence intervals.



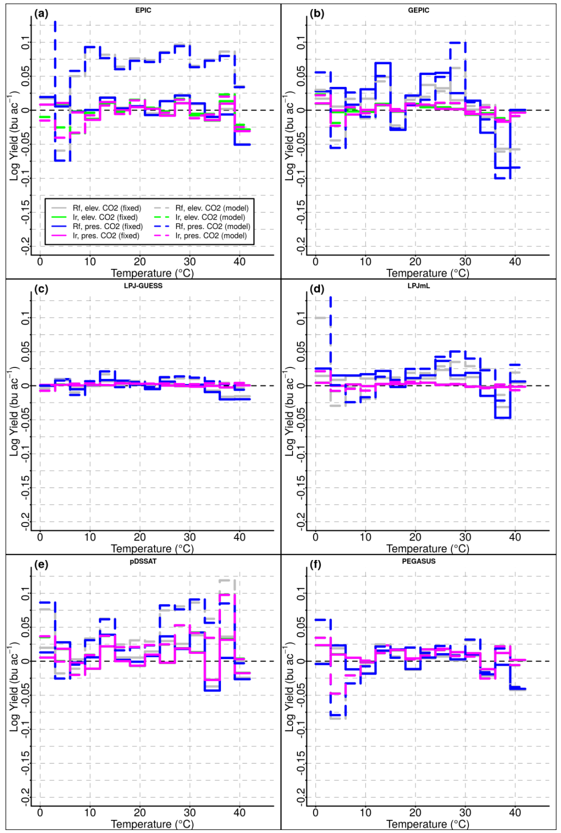
Supplementary Figure 16: US county irrigation classifications for maize **(a)**, soybean **(b)** and wheat **(c)**. The type of rainfed wheat is indicated in panel **(d)**; a threshold of 90% is used to define purely winter or spring wheat counties, respectively. Numbers below the histograms are county counts (of 3,086 in total). Counties were classified as 'rainfed' or 'irrigated' if the crop-specific share of agricultural practice in this county was at least 90% (rainfed) or 75% (irrigated), respectively; all others were classified as 'mixed'. Counties with no harvested area of the respective crop are stated as 'No cropping'.



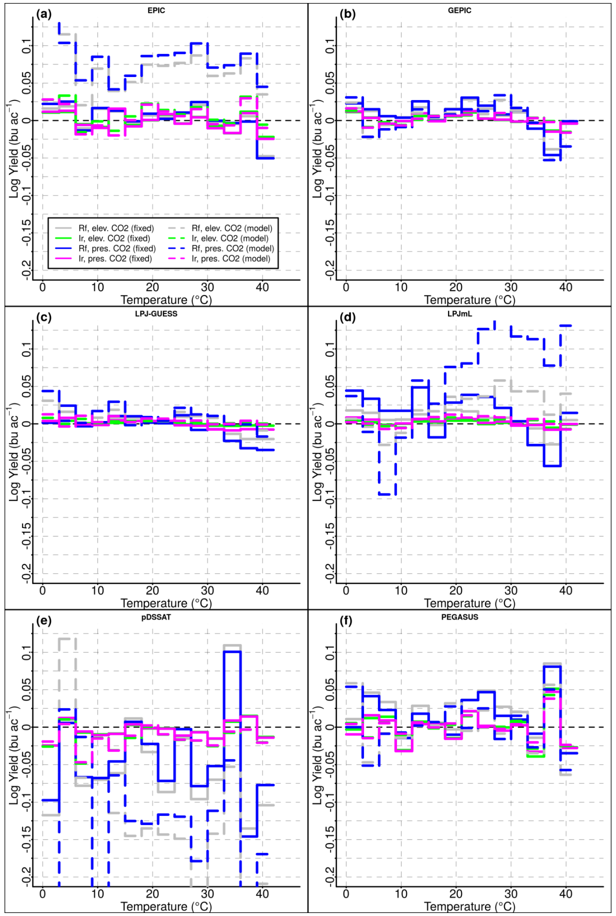
Supplementary Figure 17: Actual evapotranspiration over the historical growing season for the three crops maize, soybean and wheat under irrigated and rainfed conditions. All pairwise t-tests for mean difference are highly significant (p = 0); relative differences are shown in Supplementary Table 3.



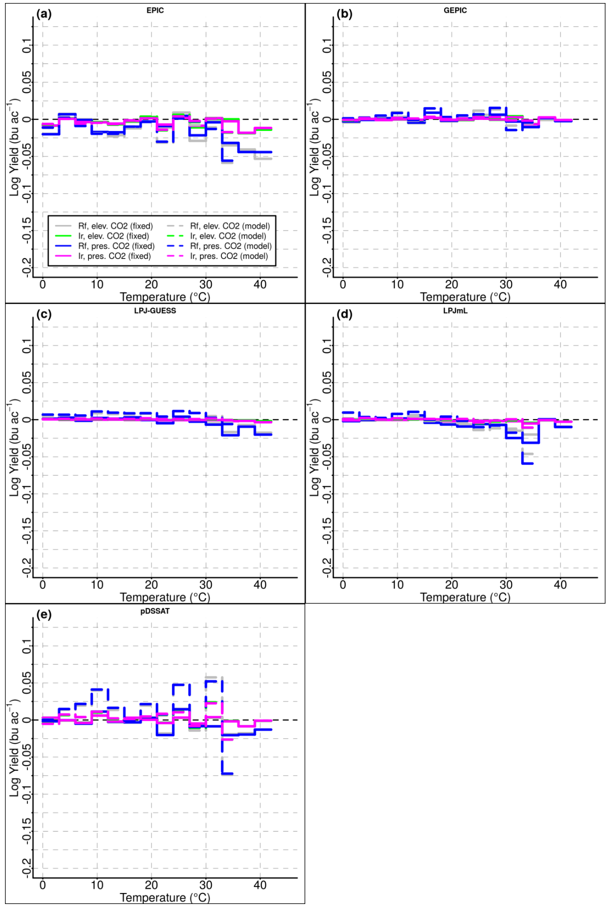
Supplementary Figure 18: Biomass accumulation over the historical growing season for the three crops maize, soybean and wheat under irrigated and rainfed conditions. All pairwise t-tests for mean difference are highly significant (p = 0); relative differences are shown in Supplementary Table 3.



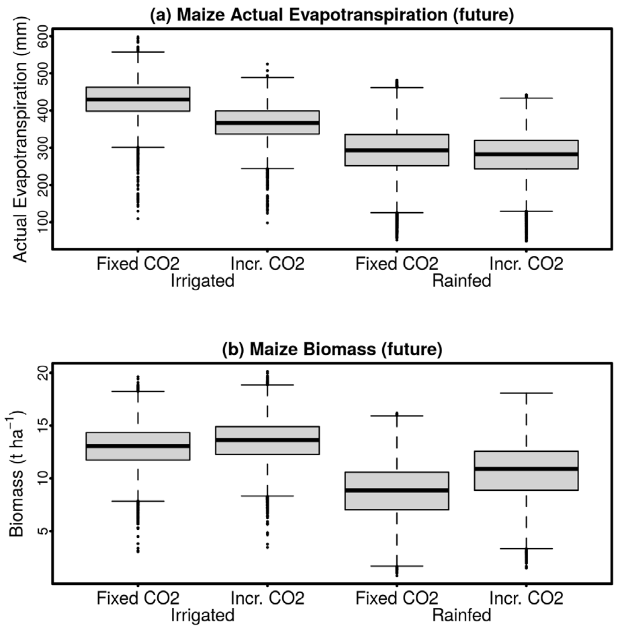
Supplementary Figure 19: Regression results for the future simulations from individual models of US maize in rainfed counties. Panels are EPIC-Boku **(a)**, GEPIC **(b)**, LPJ-GUESS **(c)**, LPJmL **(d)**, pDSSAT **(e)** and PEGASUS **(f)** models, respectively. Growing season has either been fixed from March 01 to August 31 ('fixed') or been taken from the simulation models ('model'). Confidence intervals are not drawn for visual clarity.



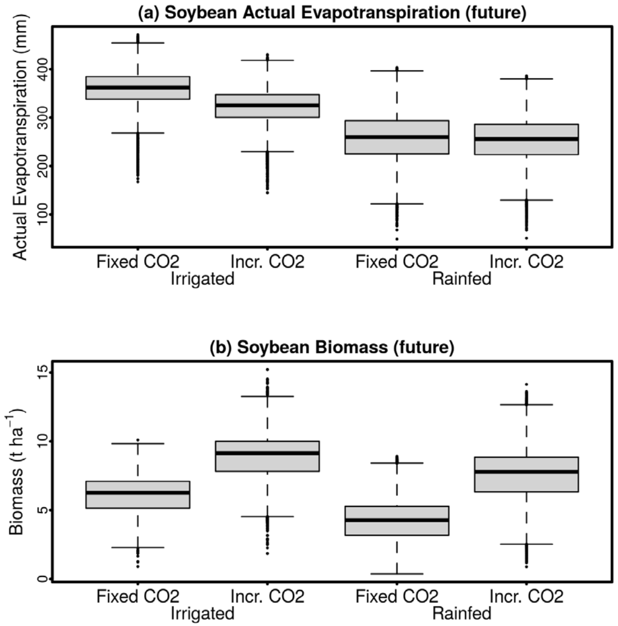
Supplementary Figure 20: Regression results for future simulations from individual models of US soybean in rainfed counties. Colors are as in Supplementary Figure 19.



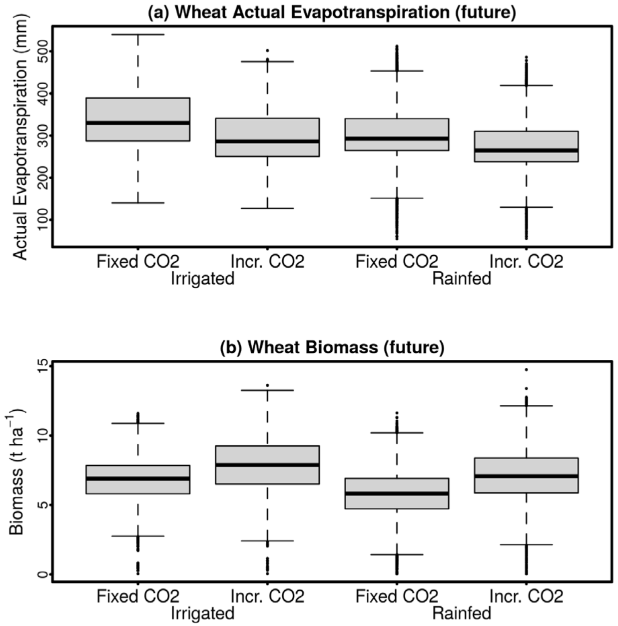
Supplementary Figure 21: Regression results for future simulations from individual models of US wheat in rainfed counties. Colors are as in Supplementary Figure 19.



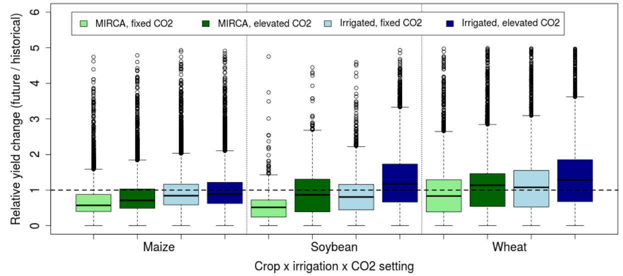
Supplementary Figure 22: Actual evapotranspiration **(a)** and biomass **(b)** over the future growing seasons for maize under four different irrigation (irrigated/rainfed) and [CO_2] (fixed present/increased) combinations. All pairwise t-tests for mean difference are highly significant (p = 0); relative differences are shown in Supplementary Table 4.



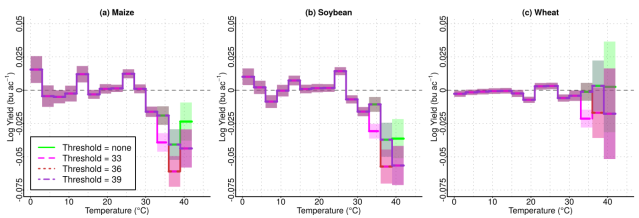
Supplementary Figure 23: Actual evapotranspiration **(a)** and biomass **(b)** over the future growing seasons for soybean under four different irrigation (irrigated/rainfed) and [CO_2] (fixed present/increased) combinations. All pairwise t-tests for mean difference are highly significant (p = 0); relative differences are shown in Supplementary Table 4.



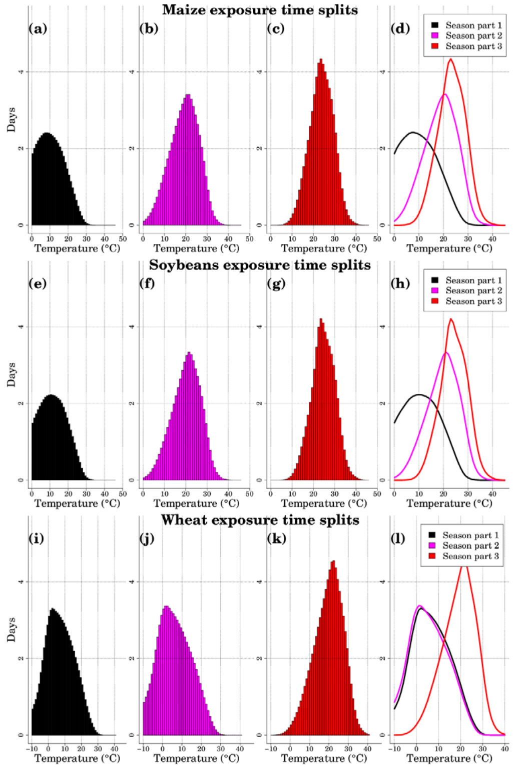
Supplementary Figure 24: Actual evapotranspiration **(a)** and biomass **(b)** over the future growing seasons for wheat under four different irrigation (irrigated/rainfed) and [CO_2] (fixed present/increased) combinations. All pairwise t-tests for mean difference are highly significant (p = 0); relative differences are shown in Supplementary Table 4.



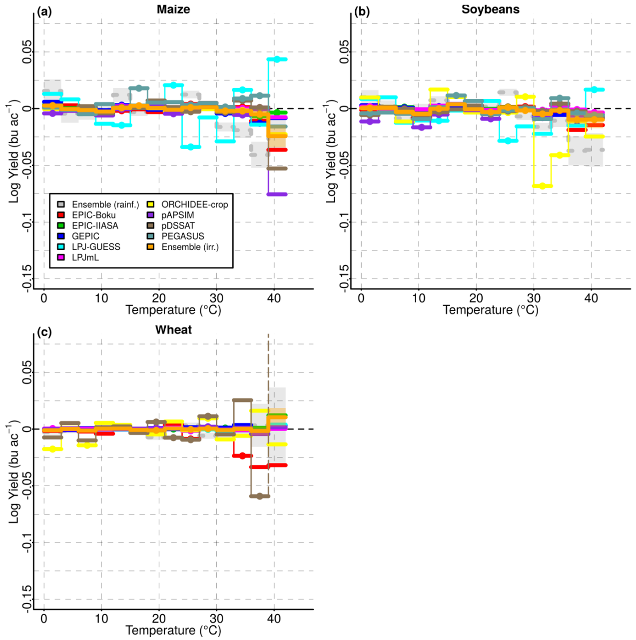
Supplementary Figure 25: Relative changes in time-averaged county yields between future and historical periods. Comparisons are individual for each crop model, but summarized in boxplots. A value of 1.0 (horizontal dashed line) indicates no change. "MIRCA" is the current irrigation pattern, and "Irrigated" is full irrigation on all cultivated areas. Outliers above 5 were removed for visual clarity (0.4% of the data). Only counties were considered where yields were available for both historical and future simulations (removed 24% of the data).



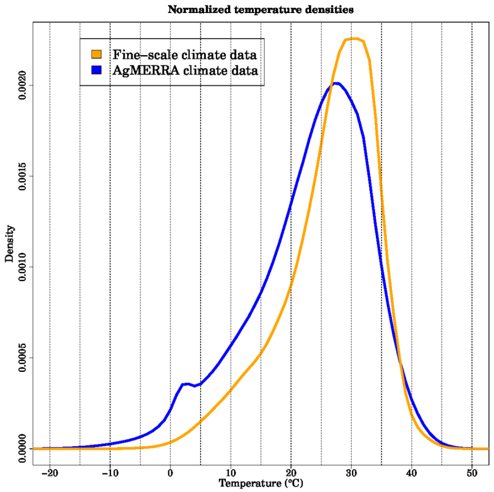
Supplementary Figure 26: Sensitivity of the statistical model to artificial yield losses from extremely high temperatures. Panels are maize **(a)**, soybean **(b)** and wheat **(c)**. Shaded areas are 95% confidence intervals. Different colors denote different temperature thresholds for yield reduction. Green curves (no reduction) are equal to green curves in Figure 1 of the main paper.



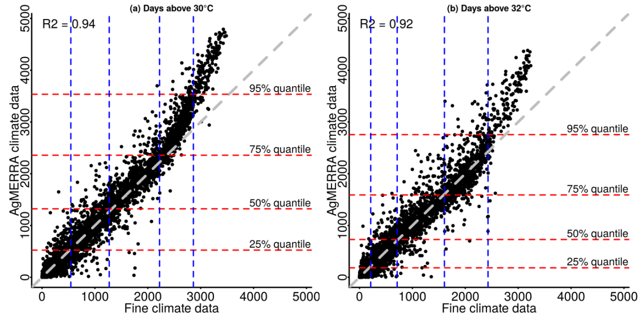
Supplementary Figure 27: Exposure times to 1°C bins during different parts of the historical fixed growing season. Panels show maize **(a-d)**, soybean **(e-h)** and wheat **(i-l)** exposure time distributions. Panels **a-c, e-g, i-k** display the temperature exposure in days for each third of the growing season . The three histograms are combined in panels **d,h,l**. The crop-specific fixed growing season is split into three equally sized parts. For maize and soybean these are March-April (part 1), May-June (part 2) and July-August (part 3). For wheat the parts are October-January (part 1), January-April (part 2) and April to July (part 3); months are split on day 15 as the fixed winter growing season is from October 15 to July 15.



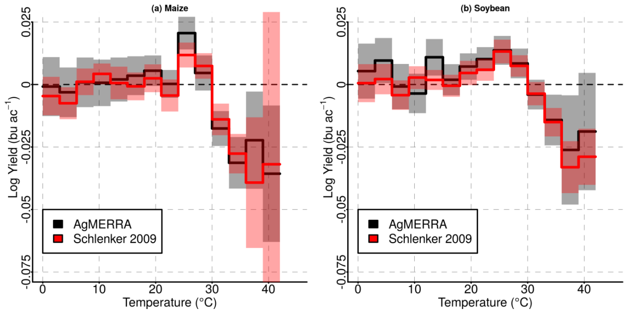
Supplementary Figure 28: Regression coefficients for US yields of individual models. Panels are **(a)** maize, **(b)** soybean and **(c)** wheat. Only US counties with predominantly rainfed agriculture are considered, but simulated yields are fully irrigated (colored lines). The dashed grey line shows coefficients from the 'rainfed' simulation ensemble (not from the observed yields) for comparison. Colored lines denote different models; the orange line is the irrigated ensemble.



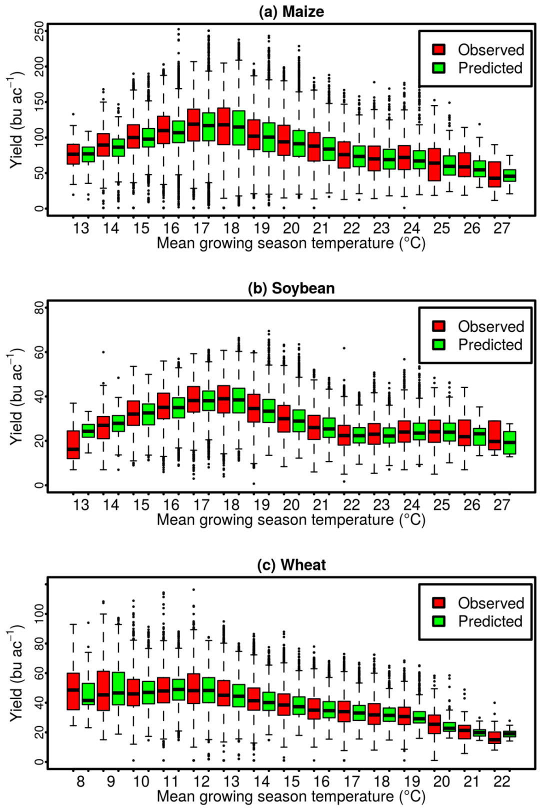
Supplementary Figure 29: Normalized frequency distribution of daily maximum temperatures as derived from the two observational climate data sets used in this study (yellow: temperature data used in the original study by Schlenker & Roberts[2] with a spatial resolution of about 0.04° x 0.04°; blue: temperature data from the AgMERRA data set used in our study and applied to force the crop model simulations with a spatial resolution of 0.5° x 0.5°). The distributions are based on the sample of all daily maximum temperatures across all grid cells without spatial or temporal aggregation. No land-use weighting has been applied.



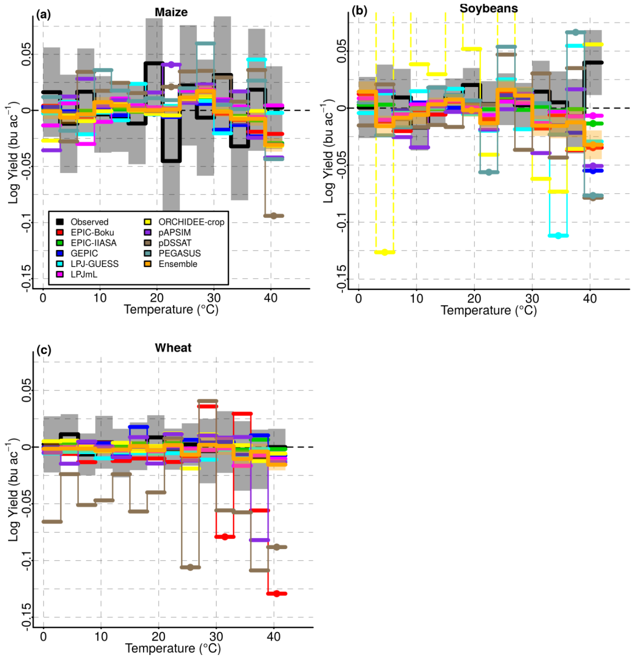
Supplementary Figure 30: Comparison of days with maximum temperature above 30°C (panel **a**) or 32°C (**b**) in all growing seasons from 1980 to 2010 for both data sets in the whole US. The x axis contains the number of days for the fine-scale climate data, while the y-axis contains the corresponding number of days for the AgMERRA climate data. Each dot corresponds to one 0.5° spatial grid cell. Red dashed lines indicate quantiles derived from the AgMERRA climate data and blue lines for the fine-scale climate data. The R^2 values in the top left corner indicate the squared correlation coefficient. Day counts for the fine-scale climate data have been computed for each 2.5-mile grid cell and then this number has been averaged within each 0.5° grid cell.



Supplementary Figure 31: Comparison of yield responses to temperature at different spatial resolutions. Maize is shown in panel **(a)** and soybean in panel **(b)**. Red lines: Temperature-bin specific coefficients γ as derived by Schlenker & Roberts[2] from the panel of all US counties east of the 100° meridian based on very high resolution temperature data (similar to Figure 1 of their paper). Black lines: Analogous analysis of the same panel data but based on the lower resolution AgMERRA data. Shaded areas are 99.5% confidence intervals.



Supplementary Figure 32: Comparison of observed and predicted yields from the regression model against mean growing season temperature. Panels are rainfed maize (a), soybean (b) and wheat (c). Observed yields are shown in red, while predicted yields are shown in green. The box plots show the median (black line within the box) and the first and third quartile (boxes). Whiskers extend to approx. the 1.6-times interquartile range and outliers are drawn with circles.



Supplementary Figure 33: Comparison of simulated to observed US yield responses to increasing temperatures for irrigated maize **(a)**, soybean **(b)** and wheat **(c)** in predominantly irrigated counties. A county is considered as predominantly irrigated if its share of irrigated agriculture exceeds 75%. Coefficients from simulated yields are marked with a dot if they significantly deviate from the observed response.

Supplementary Tables

Supplementary Table 1: Summary of basic model characteristics that could explain yield decreases under elevated temperatures. Although the models essentially consider the same effects, the mechanistic form and the parameter choices are often highly distinct between models[1, 3].

Model	Damage to enzymes/ tissues	Increasing water demand	Decreasing water supply[a]	Increasing respiration with stress	Oxidative stress (ROS)	Impaired flowering	Hastened develop-ment	Increasing root growth under water stress
EPIC-Boku	No	Yes	Yes	Yes, only T[b]	No	No	Yes	Yes
EPIC-IIASA	No	Yes	Yes	Yes, only T[b]	No	No	Yes	Yes
GEPIC	No	Yes	Yes	Yes, only T[b]	No	No	Yes	Yes
LPJ-GUESS	No	Yes	Yes	Yes, only T[b]	No	No	Limited	Yes
LPJmL	No	Yes	Yes	Yes, only T[b]	No	No	Yes	Yes
ORCHIDEE-crop	No	Yes	Yes	Yes, only T[b]	No	No	Yes	Yes
pAPSIM	No	Yes	Yes	No, but RUE* decreases	No	No	Yes	No
pDSSAT	No	Yes	Yes	Soybean: Yes, only T[b] Maize/Wheat: as pAPSIM	No	No	Yes	Yes
PEGASUS	No	Yes	Yes	No, but RUE* decreases	No	Yes[4]	Yes	Yes

[a] *Decreasing water supply means the long-term effect of an increasing atmospheric demand, i.e. water that is consumed by evapotranspiration now is not available from the soil later*
[b] *"only T" means that respiration is only influenced by temperature, but not by water supply*

Supplementary Table 2: Implementation of CO_2 effects in the nine models. The effect of these implementations has been assessed in a separate study[5].

Model	CO_2 effects*
EPIC-Boku	RUE, TE
EPIC-IIASA	RUE, TE
GEPIC	RUE, TE
LPJ-GUESS	LF, SC
LPJmL	LF, SC
ORCHIDEE-crop	LF, SC
pAPSIM	RUE, TE
pDSSAT	RUE, TE (maize, wheat), LF (soybean)
PEGASUS	RUE, TE

** LF = Leaf-level photosynthesis (via Rubisco or quantum-efficiency and leaf-photosynthesis saturation)*
RUE = Radiation use efficiency
SC = Stomatal conductance
TE = Transpiration efficiency

Supplementary Table 3: Relative differences between irrigated and rainfed AET and biomass medians for maize, soybean and wheat over the historical growing season. Differences are reported relative to the median value of the pooled samples for each crop.

Variable	Crop	Relative difference rainfed / irrigated (in %)
AET	Maize	14.8
	Soybean	20.0
	Wheat	21.6
Biomass	Maize	24.9
	Soybean	33.7
	Wheat	13.8

Supplementary Table 4: Relative differences between irrigated/rainfed and fixed present/elevated CO_2 concentrations in AET and biomass medians for maize, soybean and wheat over the future growing season. Differences are reported relative to the median value for the pairwise pooled samples. Abbreviations: rf = rainfed, ir = irrigated, CO_2- = fixed present, CO_2+ = elevated concentration.

Variable	Crop	Relative differences (in %)			
		rf / ir with CO_2-	rf / ir with CO_2+	CO_2-/CO_2+ with ir	CO_2-/CO_2+ with rf
AET	Maize	41.0	27.0	20.2	3.4
	Soybean	35.7	25.3	13.2	1.4
	Wheat	12.5	7.9	16.4	10.4
Biomass	Maize	41.0	22.8	4.6	17.1
	Soybean	41.4	16.6	35.2	43.1
	Wheat	17.8	11.2	13.5	17.2

Supplementary Table 5: Decline in length of growing season (days) for each additional degree of mean growing season temperature. Coefficients are averaged over all individual county slopes for the respective setting (*crop* x *model* x *water supply*).

Crop	Model	Rainfed	Irrigated
Maize	EPIC-Boku	NA[a]	NA[a]
	EPIC-IIASA	-9.1	-9.0
	GEPIC	-9.4	-9.5
	LPJ-GUESS	-9.0	-9.1
	LPJmL	-12.0	-11.4
	ORCHIDEE-crop	-3.7	-5.0
	pAPSIM	-4.6	-4.5
	pDSSAT	-7.4	-6.7
	PEGASUS	-4.0	-4.0
	Model average	***-7.4***	***-7.4***
Soybean	EPIC-Boku	NA[a]	NA[a]
	EPIC-IIASA	-6.3	-6.8
	GEPIC	-9.6	-9.6
	LPJ-GUESS	-5.3	-7.0
	LPJmL	-9.0	-9.4
	ORCHIDEE-crop	-3.5	-5.6
	pAPSIM	-3.5	-3.6
	pDSSAT	-2.3	-1.3
	PEGASUS	-5.6	-5.6
	Model average	***-5.6***	***-6.1***
Wheat	EPIC-Boku	NA[a]	NA[a]
	EPIC-IIASA	-2.6	-3.3
	GEPIC	-6.1	-4.4
	LPJ-GUESS	-1.8	-4.8
	LPJmL	3.8	-3.0
	ORCHIDEE-crop	NA	-9.0
	pAPSIM	0.5	9.5
	pDSSAT	-1.4	1.7
	Model average	***-1.3***	***-1.9***

[a] *EPIC-Boku did not provide model-specific growing seasons in the simulations used.*

Supplementary Notes

Supplementary Note 1 – Robustness of the regression approach

The regression approach does not suffer from the rather large number of explanatory variables (approx. 80 for rainfed counties). A similar response of yields to temperature can be obtained with a so-called "piecewise-linear" approach, following the ideas by Schlenker & Roberts[2], where only two temperature parameters are fitted (Supplementary Figures 1-3)). Additionally, a modified Principal-Component-Regression yields no different results than the multiple linear regression applied in the main paper (Supplementary Figure 4). This proves that multi-collinearity between the temperature exposure times is not influencing the regression results. Altogether there is ample evidence for trusting in a robust temperature response of yields in the analyzed setup, since the results do not critically depend on the regression method chosen or the number of its parameters.

The piecewise linear approach, as introduced by Schlenker & Roberts[2], performs a regression of yields against growing degree days, accumulated over the growing season. Two fixed end points at 8 and 40°C (0 and 40°C for wheat) frame the crop's response; an endogenous threshold up to which temperature affects yields positively, and above negatively, is found by looping over all possible thresholds between 15 and 35°C (maize and soybean) or 6 and 35°C (wheat) and choosing the one (threshold plus associated slopes) with the highest R^2. For more details of the method please refer to ref. [2]. This piecewise linear approach, where only two temperature-dependent slopes are estimated, exhibits the same yield response as the step-function regression applied in the main paper – which indicates that the response is stable and independent from the regression method.

A modified Principal-Component-Regression was applied to the data set to control for multicollinearity between temperature variables. We kept precipitation, county-fixed effects and state-time trends in the data matrix, but selected only those temperature bins that a principal component analysis yielded as most important (a standard deviation larger than two was used as cutoff, then representative temperature variables were selected for each component). Afterwards the standard multiple regression analysis as described in the main paper was applied to the reduced data set. For all crops the temperature coefficients are comparable to the original regression results (Supplementary Figure 4). Note that a 'classical' Principal-Component regression of *all* explanatory variables (i.e. regressing yield on transformed orthogonal components) yields similar results, but does not provide information on standard errors – this is why we resorted to the modified approach.

Supplementary Note 2 – Responses for individual models

Of the 26 crop x model cases (9 for maize, 9 for soybean, 8 for wheat) the general temperature response pattern of the rainfed observed yields is captured in 21 cases. But there are five cases where the simulated rainfed temperature response pattern strongly differs from the observed one for rainfed yields: LPJ-GUESS for maize and soybean, ORCHIDEE-crop for soybean and wheat and EPIC-Boku for wheat. The likely reason for the unexpected response is a low average yield. ORCHIDEE-crop simulates only between 34-68% of the ensemble mean yields for all three crops, LPJ-GUESS simulates 51-68% of mean yields for maize and soybean (but 117% for wheat) and EPIC-Boku simulates 67% of mean yields for wheat. The low average yields seem to reduce the signal-to-noise ratio through an increased coefficient of variation, which results in an unexpected temperature response.

Supplementary Note 3 – Coefficient correlations

To enhance visibility of coefficient differences we correlate coefficients estimated from observed and simulated yields. For each crop and irrigation setting in rainfed counties the regression coefficients γ_h from simulated yields are compared in a 1:1 plot with coefficients from observed yields. Qualitative differences between the coefficients for rainfed and irrigated yields can be seen for both maize (Supplementary Figure 13) and soybean (Supplementary Figure 15), in particular for the negative observed ones. But for wheat there is no pattern in the difference between the correlations of either rainfed or irrigated simulated yields with the observed rainfed coefficients (Supplementary Figure 14) – which confirms that there is no detectable response of historical wheat yields to high temperature. These plots are useful for telling whether there is a difference between irrigated and rainfed yield responses, for all coefficients at once rather than for single coefficients. The R^2 correlation values (in the legends) are inconclusive for the modelling capacity as there is little difference between the rainfed and the irrigated comparisons, due to the close clustering of values around 0.

Supplementary Note 4 – Model results in irrigated counties

Regression coefficients if only irrigated (fraction >75%) counties are chosen are shown in Supplementary Figure 33. There is no pattern in the response of observed yields to temperature; all coefficients (except one for maize and two for soybean) are insignificant. The yield drop at elevated temperatures above 30°C is absent in particular for maize and soybean. The positive coefficient for soybean at temperatures above 39°C may be a

regression artefact due to few days with this temperature and the insignificance of 12 of the other 13 coefficients, but does not contradict our findings. The negative responses of pDSSAT wheat (panel c, brown curve) to all except two temperature bins are insignificant (confidence intervals contain 0) and underline the independence of irrigated yields from temperature. Additionally, the sample size for irrigated wheat is small with only 10 counties in Arizona containing sufficient data. Why pDSSAT responds differently than the other models in this case has not been investigated here but would require further data on irrigated wheat.
The models generally show a slightly higher responsiveness to temperature than the observations do. This might indicate that some management decisions apart from irrigation are reflected in the observed but not in the simulated yields.

Supplementary Note 5 – Sensitivity of the regression to extreme heat

The low relative abundance of extremely high temperatures above 36°C could lead to a lower sensitivity of the statistical model to detect yield effects of these temperatures. We tested this sensitivity by artificially reducing simulated yields at each grid cell for each day above different temperature thresholds. We used 33, 36 and 39°C as thresholds, above which each day reduced crop yields by 2%. Thus, 10 days at e.g. 33°C or above reduce crop yields by a factor of 0.98^10 = 0.817. The reduction was additionally applied to simulated historical ensemble yields in rainfed counties. Reductions were applied to yields in grid cells and then aggregated to counties.
The statistical approach shows correct quantitative responses to artificially induced "temperature stress" by log(0.98) = -0.02 lower coefficients at and above the thresholds (Supplementary Figure 25). Thus we conclude that the regression is sensitive to extremely high temperatures, independent of their relative abundance, and that the aggregating from grid cells to counties does not conceal these events. All coefficients below the threshold temperatures are unchanged, which shows the robustness of the approach and the specificity towards temperature bins.

The distribution of exposure times differs across different parts of the historical growing season (Supplementary Figure 26). Earlier parts of the (fixed) growing season contain cooler average temperatures and less high temperature events. Most of the high (above 30°C) and extremely high (above 36°C) temperature events expectably occur in the last part of the growing season. But for maize and soybean already a substantial number of these events occur in the middle part of the growing season. For wheat high temperature events occur only in the third part. It is evident that many crops experience (extremely) high temperatures already in the middle part of the growing season. Crop anthesis dates for maize (June/July), soybean (June/July) and wheat (May) usually lie at the end of part 2 or in

part 3 of the growing season[1]. Grain filling mostly occurs in the last part, which experiences the highest temperatures. Both anthesis and grain filling are known to be very sensitive to high temperatures[6, 7, 8, 9, 10, 11, 12]. Thus, effects of extreme temperatures do not seem to be underestimated by extremely high temperatures only occurring in insensitive phases of the season. A sensitivity test towards the definition of the growing season and the timing of the exposure to high temperatures has already been performed by Schlenker & Roberts[2], resulting in qualitatively and quantitatively the same responses as for the full season.

Supplementary Note 6 – Appropriateness of the climate data

The AgMERRA[13] climate data used in this study are one order of magnitude coarser (0.5° x 0.5°) than those used by Schlenker & Roberts at a 2.5-mile resolution (about 0.04°)[2]. We decided to use the AgMERRA data instead as the GGCMs from the AgMIP ensemble were also forced by them. The temperature distribution of the fine-scale data set is slightly shifted with lower densities below about 27°C and higher densities in the temperature range from 27°C to 37°C (Supplementary Figure 29). The fine-scale climate data are constructed from monthly and daily data; this is described in the supplement of Schlenker & Roberts[2]. The comparison between the two climate data sets therefore shows differences between these, but not necessarily differences between AgMERRA and the "true" climate.

We also analyzed the spatial agreement of the two temperature distributions by comparing the numbers of days with maximum temperature above certain thresholds (30°C and 32°C) for each individual 0.5° grid cell. For each cell the days within all growing seasons (March 01 till August 31) from 1980 to 2010 above these thresholds are accumulated. Day counts for the fine-scale climate data are averaged for each 0.5° grid cell, which follows a similar consideration as in Schlenker & Roberts, but could still result in a flattening of extreme outlier values. The resulting day counts correspond closely (Supplementary Figure 30, one dot corresponds to one grid cell), with R^2 values of 94% and 91%, respectively. The AgMERRA data tend to include even more hot days than the fine-scale climate data in the very hot regions.

To test the sensitivity of the coefficients to the deviations of the temperature distributions we compare our scaling coefficients based on the AgMERRA data to the ones originally derived by Schlenker & Roberts. Both estimates for observed rainfed yields agree closely (Supplementary Figure 31), in particular also in the temperature range above 30°C. There is no hint for a significant divergence of the regression coefficients based on the higher resolution temperatures and the ones based on the AgMERRA data for both maize and

[1] http://www.usda.gov/oce/weather/pubs/Other/MWCACP/MajorWorldCropAreas.pdf ; accessed on August 23, 2016

soybean (the two crops considered by both Schlenker & Roberts and also simulated by our ensemble of GGCMs).

The rainfed yields predicted from the regression model (equation 1 in the main paper) based on the AgMERRA data agree closely with the rainfed observed yields (Supplementary Figure 32). Observed and predicted yields are plotted against mean growing season temperature for maize (panel a), soybean (panel b) and wheat (panel c). Observed yields are in red, while yields predicted by the regression model are in green.

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5 A global semi-empirical model for yield anomalies and yield forecasting

This chapter is a reformatted reproduction of the article published as "Schauberger, Gornott & Wechsung: Global evaluation of a semi-empirical model for yield anomalies and application to within-season yield forecasting, Global Change Biology, June 2017" at John Wiley and Sons. The article DOI is 10.1111/gcb.13738.

5.1 Article

ABSTRACT

Quantifying the influence of weather on yield variability is decisive for agricultural management under current and future climate anomalies. We extended an existing semi-empirical modeling scheme that allows for such quantification. Yield anomalies, measured as inter-annual differences, were modeled for maize, soybeans and wheat in the US and 32 other main producer countries. We used two yield data sets, one derived from reported yields and the other from a global yield data set deduced from remote sensing. We assessed the capacity of the model to forecast yields within the growing season.

In the US, our model can explain at least two thirds (63-81%) of observed yield anomalies. Its out-of-sample performance (34-55%) suggests a robust yield projection capacity when applied to unknown weather. Out-of-sample performance is lower when using remote-sensing derived yield data. The share of weather-driven yield fluctuation varies spatially, and estimated coefficients agree with expectations. Globally, the explained variance in yield anomalies based on the remote-sensing data set is similar to the US (71-84%). But the out-of-sample performance is lower (15-42%). The performance discrepancy is likely due to shortcomings of the remote-sensing yield data since it diminishes when using reported yield anomalies instead. Our model allows for robust forecasting of yields up to two months before harvest for several main producer countries. An additional experiment suggests moderate yield losses under mean warming, assuming no major changes in temperature extremes.

We conclude that our model can detect weather influences on yield anomalies and project yields with unknown weather. It requires only monthly input data and has a low computational demand. Its within-season yield forecasting capacity provides a basis for practical applications like local adaptation planning. Our study underlines high-quality yield monitoring and statistics as critical prerequisites to guide adaptation under climate change.

INTRODUCTION

Strongly varying crop yields can endanger farmers' livelihoods and can lead to national production shortages. Yields are determined by weather and agronomic management influences as well as by stress factors like pests or diseases. For calculating crop yields under current or a changing climate it is important to quantify these influences. Therefore we devise a semi-empirical modeling scheme which allows for quantifying weather influences with high explained variance. We use two different yield data sets with different qualities, one based on reported yield data and the other on remote sensing combined with yield statistics. We show the ability of the model to predict yield anomalies up to two months before harvest.

Two approaches are widely used to simulate crop yields (Di Paola *et al.*, 2016, Jones *et al.*, 2016, Lobell & Burke, 2010). Process-based models simulate physiological processes like carbon assimilation to calculate yields. Statistical models correlate yields with yield-determining factors to elicit contributions of individual factors. Both approaches, and hybrids between them, can aid in understanding and forecasting weather-related yield variability (Liu *et al.*, 2016). Their application to conditions (e.g. climate) out of the training scope is a contested area, however (Lobell & Burke, 2010, Rötter *et al.*, 2011).

Here we extend an existing statistical framework for modeling inter-annual yield variability. The approach is "semi"-empirical as known physiological influences are reflected in the exogenous variables, following the naming of Rahmstorf (2007). The concept was introduced in Wechsung *et al.* (2008) and later successfully applied to German maize and winter wheat yields (Gornott & Wechsung, 2016). We extend the model by adding temperature-stress related variables, using more crops, applying it to 34 countries and providing two application cases: forecasting yield anomalies up to two months before harvest and gauging of yield losses under moderately increased temperatures.

We analyze four staple crops: maize, wheat (spring and winter separately) and soybeans, which cover approx. 34% of the global harvested area (Portmann *et al.*, 2010). We use reported crop yield data in seven countries and a global gridded yield data set that downscaled reported yield statistics utilizing satellite data (here used for 33 countries). Subnational yield data are needed for quantifying spatial differences of yield influences. Though these data are increasingly available, there are still data-scarce regions especially in developing countries. The global and publicly available data set supplied by Iizumi *et al.* (2013b) might serve as alternative. The dataset uses annual remote sensing information to downscale national and subnational yield statistics. The algorithms utilized therein to separate reflectance data spatially and temporally into crops or vegetation necessarily introduce uncertainty, which increases with the share of other vegetation types in grid cells. Despite these caveats we test the potential of this global gridded data set for quantifying yield anomalies, as it may be helpful when subnational yield data are not accessible.

We apply a two-step procedure: the model performance is first analyzed in depth in the US and then, second, extended to all main producing nations. We start with US yields, since the high-quality yield data base curated by the US Department of Agriculture (USDA, 2015) allows for rigorous model evaluation. The model is applied in parallel to the USDA and the Iizumi *et al.* (2013b) data. The US are one of the largest crop producers (FAO, 2016) and have highly diverse climate and soils. We employ one model specification based on selection results by Gornott and Wechsung (2016), but test its sensitivity regarding variations in yield-influencing factors and transformation of variables. Additionally, we include penalty terms for heat and frost.

Instead of absolute yields we consider yield anomalies to remove trends, systematic biases and time-invariant farm- or county-specific influencing factors. Normalizing anomalies of yield and exogenous variables by the logarithm allows a comparison of influences across scales and variables. Only weather variables are included in the model, explicitly neglecting agronomic influences like acreage, shifting land use or fertilizer application on inter-annual yield fluctuation (Mueller *et al.*, 2012, Ray *et al.*, 2015). But these data do not increase model performance in Germany (Conradt *et al.*, 2016) and are difficult to obtain as time series on a spatially explicit level with large spatial coverage; they would therefore enlarge uncertainty. We only use monthly weather values which are deemed to provide more reliable information than daily weather data from models due to aggregation effects (Kilsby *et al.*, 2007, Lobell, 2013, Maurer *et al.*, 2010). This also avoids the use of downscaling methods when using climate model outputs (Glotter *et al.*, 2014, Iizumi *et al.*, 2012).

MATERIALS AND METHODS

Input data

<u>Yield data</u>

We employed two sets of yield data for maize, soybeans, spring and winter wheat (all in t/ha). For the US we used either USDA (USDA, 2015) yields at county level, from 1980 to 2010, or gridded yield data from Iizumi *et al.* (2013b) from 1982 to 2006 (henceforth "GGYD" for "Gridded Global Yield Data"). Both were re-gridded to 0.5° spatial resolution (about 50 km at the equator) to match with the resolution of the weather and land-use data. USDA county yields were assigned to each 0.5° grid cell that completely fall within a county or intersect with its boundaries; yields for grid cells intersecting with several counties were averaged. GGYD yields are provided at 1.125° resolution and were interpolated to 0.5° with second order conservative remapping (preserving fluxes and spatial gradients). Additional county-level yields for Germany, Russia, Tanzania, Australia, Brazil and Burkina Faso (from the respective statistical offices) allowed for further model and yield data quality assessments. National yield time series from FAO (FAO, 2016) were used for comparison of aggregated yield time series. We considered those countries as main producers (Figure 1, SI Table S3) which, sorted by total production, together accounted for more than 90% of world production for a specific crop between 2000 and 2011 (FAO, 2016).

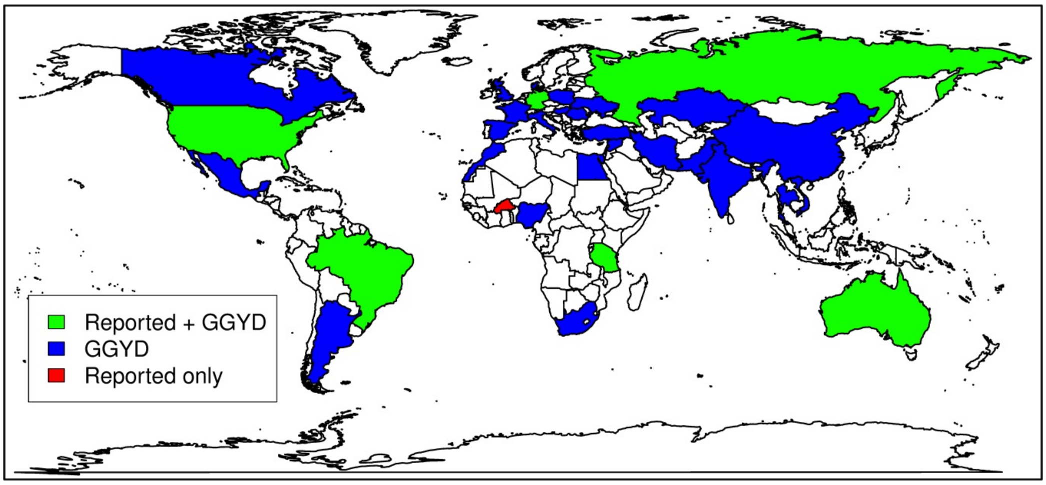

***Figure 1**: World map of countries analyzed in this study. Colors of countries denote whether GGYD and reported yields (green), only GGYD yields (blue) or only reported yields (red) are used in this study. Countries in white are no main producers and not analyzed.*

Weather data

We used AgMERRA climate data (Ruane *et al.*, 2015) at 0.5° spatial and monthly temporal resolution, providing minimum, maximum and average temperature, precipitation and shortwave radiation from 1980 to 2010. AgMERRA has been designed for use in agricultural research focusing on reproducing both average and extreme values.

Growing season and land-use data

We utilized static MIRCA2000 crop- and irrigation-specific land-use fractions around 2000 on 0.5° spatial resolution (Portmann *et al.*, 2010). Growing seasons were also taken from MIRCA2000, using the sub-crop with the largest harvested area. Winter and spring wheat were distinguished by their growing season length: eight or more months were classified as winter wheat, four months or less as spring wheat. Remaining ambiguities were resolved by considering the sub-crop with the maximum (minimum) growing season length as winter (spring) wheat. Soybeans have a prolonged flowering period (Ritchie *et al.*, 1993) at the transition between vegetative and reproductive season. Although it could be physiologically reasonable, we restrained from reflecting this period in a separate set of exogenous variables to avoid collinearities and rank deficiencies (many variables for few data).

Regression scheme

Definition

We applied an ordinary least squares (OLS) regression scheme based on the Cobb-Douglas production function with different model specifications. The function relates inter-annual changes of crop yields to a product of inter-annual changes of weather variables (equation 1; SI equation SE3). The natural logarithm linearizes all terms into a sum.

$$\log y_t{}' = \log \beta_0 + \sum_{j=1}^{J} \beta_j \log x'_{jt} + \log u'_t \text{ , with } j = 1, \dots, J \text{ and } t = 1, \dots, M \qquad \text{(eq. 1)}$$

Variables are yield (y), weather (x_j) and error term (u). Estimated coefficients are $\beta_{0..J}$ and denote intercept (β_0) and weather influences. All variables are provided per grid cell. Years are indexed with t. Anomalies are denoted with a prime ($'$). We calculated yield anomalies as first differences ($y'_t = y_t - y_{t-1}$) between adjacent years, making an explicit time variable obsolete. We used two regression methods: STSM (Separate Time Series Model) and PDM

(Panel Data Model). While STSM estimates an independent model for each grid cell, the PDM parametrizes relationships across grid cells, allowing for spatial variation in mean yields with grid cell-specific fixed effects. These choices are justified by earlier results (Conradt *et al.*, 2016, Gornott & Wechsung, 2016) and the similarity of results under different techniques (SI Section 3). Whether spatial correlation poses a problem for the PDM method is tested (see below). In the US we considered nine climatic regions (SI Figures S1-2). Other, larger main producers were split into administrative boundaries for PDM estimation; for all others only one national PDM was estimated (SI Table S3).

Exogenous variables

Exogenous variables either describe potential growth or stress factors that reduce growth, included for their known physiological relevance. They are tested for statistical significance, but the model formulation stays constant. We therefore consider the model as "semi"-empirical following the argumentation of Rahmstorf (2007). A combined temperature-radiation variable relates yields to potential growth. Temperature-normalized solar radiation (SRT, equation 2) is used to account for co-linearity in both variables. Killing (KDD) and freezing degree days (FDD) were added to better account for the non-linear influence of extreme temperatures on crop yields (Barlow *et al.*, 2015, Schlenker & Roberts, 2009). They are defined as the temperature sum above or below a crop-specific threshold, respectively (equations 3,4). The KDD threshold T^{KDD} was 32°C for all crops, while the FDD threshold T^{FDD} was -15°C for the two wheat types and 0°C for maize and soybeans (Hatfield *et al.*, 2011, Luo, 2011, Porter & Gawith, 1999, Sanchez *et al.*, 2014).

$$SRT = \frac{R_S}{T_{avg}+20} \qquad \text{(eq. 2)}$$

$$KDD = \sum_{d=1}^{N} \max(T_d - T^{KDD}; 0) \qquad \text{(eq. 3)}$$

$$FDD = \sum_{d=1}^{N} \min(T_d - T^{FDD}; 0) \qquad \text{(eq. 4)}$$

Further stress variables comprised potential evapotranspiration (PET) and precipitation. Both variables map the yield-reducing effect of inadequate demand and supply of water by PET and precipitation, respectively. PET was calculated from VPD according to Haude (1955) as in Gornott and Wechsung (2016) except that the month-specific correction factor f_H was considered constant for the sake of a simpler model. For winter wheat only the reproductive part of SRT was considered, while for the other crops only the vegetative part was used. The full regression specification is provided in SI section 2. Further agronomic justifications are provided in Gornott and Wechsung (2016). Economic variables like fertilizer price and harvested area were not considered since these only added little explanatory power in Germany (Conradt *et al.*, 2016) and are generally not available on larger areas across the world.

PET and precipitation were split between the vegetative and reproductive part of the growing season. The identification of both parts was based on phenological heat units. The first month of the reproductive period was defined as the first month where the temperature sum, accumulated over the growing season until this month, exceeds 50% of the total temperature sum, accumulated over the whole growing season (supplementary equations SE4,5).

Aggregation

After estimation yield anomaly time series (observed, predicted and one-out-of-sample predicted yield anomalies) were aggregated from grid cells to climate regions or countries (supplementary equations SE1,2). Aggregation was performed unweighted, i.e. treating each grid cell as equal, or weighted by land-use patterns according to MIRCA2000. Performance measures (see below) were then calculated for aggregated time series.

Model evaluation

Performance

Six performance indicators were calculated: coefficient of determination (R^2), root mean square error (RMSE), Nash-Sutcliffe efficiency (NSE), one-out-of-sample R^2 (henceforth: R^2_{O1}), out-of-temperature R^2 (R^2_{OOT}) and out-of-precipitation R^2 (R^2_{OOP}). The first three are standard model evaluation indices and measure the explained variance, the mean deviation and a combined measure of model bias and variability, respectively. They indicate the capacity of the model to explain yield anomalies, which is important for interpreting coefficients. R^2_{O1} was calculated by subsequently and separately stripping each year from the estimation data, estimating the model with the reduced data and eventually predicting yield anomalies for the stripped year with this reduced model. R^2_{O1} thus indicates the model's capacity to project yields from weather data that have not been used for model training. R^2_{OOT} and R^2_{OOP} were similarly calculated by omitting the six first-differences towards and from the three warmest (driest) years, defined by highest growing season mean temperature (lowest precipitation over PET). Thus the model was trained on six yield anomalies less and was then used to predict these missing anomalies. The correlation between these predicted and observed anomalies in only the warmest (driest) years, calculated across aggregation regions, indicates the capacity to project yield anomalies under warmer (drier) climate. Performance measures were calculated on nationally aggregated time series, but are also available for each grid cell.

Statistical tests

The adequacy of the linear model for capturing yield anomalies was examined with six statistical tests. The regression equation specification error test (RESET) evaluated whether quadratic variables would improve the model. The Lagrange multiplier test according to Breusch–Pagan (LM) was used to examine spatial independence of the data. The Breusch–Godfrey test was applied to assess autocorrelation and the Breusch–Pagan test to probe heteroscedasticity (Croissant & Millo, 2008, Wooldridge, 2013). Normal distribution of residuals was tested using the Shapiro–Wilk test. Whether multi-collinearity of exogenous variables poses a problem was assessed with the condition index following Belsley *et al.* (1980). All analyses were performed with R (R Core Team, 2016).

Model application

Two practical applications of the model were performed.

Yield forecasting

The model was applied to forecast yield anomalies during the growing season up to two months before harvest. We clipped the last one or two months, respectively, from the MIRCA2000-defined growing season and calculated all weather variables based on this reduced season. Afterwards the model was trained on the reduced weather data set, relating yield anomalies to weather anomalies observed up to one or two months before harvest. The one-out-of-sample performance of this reduced model is then a measure for its forecasting capacity.

<u>*Yield effects from temperature warming*</u>

Effects of moderate warming were calculated as a model application case. Temperature in every *second* growing season of the AgMERRA climate was raised by 0.9 or 1.4 °C, corresponding to the difference between the 0.6 °C of warming already present in 1986-2005 (Schleussner *et al.*, 2016) and current climate change targets of 1.5 or 2 °C. Differences in warming over land and ocean (IPCC, 2013) were neglected. Precipitation and radiation were not modified since we assume stochastic changes with mean zero for this temperature range (IPCC, 2013). Differences in CO_2 concentrations would be relevant for absolute yields, but were not considered due to rather minor changes (plus ~30 or 60 ppm for 0.9 or 1.4 °C warming, respectively, compared to 1980-2010 average concentrations; IPCC (2013)). The CO_2 increase of ~60 ppm during the historical period is not relevant for this application when assuming a similar increase in the warmed period – first differences cancel the trend in both time series. Yield anomalies were predicted with coefficients estimated from unmodified climate and exogenous variables from the artificial climate data. Grid-cell yield time series were nationally aggregated without weighting. The first-difference approach allows interpreting yield changes between adjacent years as effects of temperature increases. Yield changes (unmodified to modified and modified to unmodified years, with inverted signs) were averaged and the logarithm removed. A temperature change of 0 °C was used for deriving normalization constants with which all other yield changes were multiplied. Uncertainty of predictions u was calculated by adding RMSE of the one-out-of-sample model ($RMSE_{OI}$) and variance of the temperature-modified yield time series (eq. 5):

$$u = \sqrt{(RMSE_{O1})^2 + Var(mod.time\ series)} \quad \text{(eq. 5)}$$

RESULTS

Results for the contiguous US

The model had a substantial capacity for explaining and predicting yield anomalies. Yield anomaly time courses for USDA-based models are shown in Figure 2. Results for each of the eight crop-yield data set combinations are displayed in Table 1. All grid cells where the specific crop is grown are included. Either unweighted or weighted aggregation was used, decided on the higher R^2_{O1} for each crop individually. Time series for US regions are provided in SI Figure S11. A performance comparison of different model specifications is provided in SI Figure S6. All statistical tests indicated that the OLS model estimation is adequate (SI section 4).

***Table 1**: Model performance for eight crop-yield data set combinations in the US. Columns are crop, yield data set, application of land-use weighted aggregation, Nash-Sutcliffe efficiency (NSE), explained variance of the modeled (R^2) and one-out-of-sample time series (R^2_{O1}), out-of-temperature and out-of-precipitation correlation (R^2_{OOT} and R^2_{OOP}) and the share of grid cells for which the model is significant (p < 0.05).*

Crop	Yield data	Weighted Aggregation	NSE	R^2	R^2_{O1}	R^2_{OOT}	R^2_{OOP}	Significant Cells
Maize	USDA	No	0.74	0.81	0.55	0.31	0.11	51 %
	GGYD	No	0.70	0.92	0.59	0.08	r<0	47 %
Soybeans	USDA	No	0.69	0.69	0.45	0.38	0.02	60 %
	GGYD	Yes	0.60	0.72	0.18	r<0	r<0	24 %
Spring wheat	USDA	No	0.63	0.63	0.34	0.28	0.42	52 %
	GGYD	No	0.61	0.73	0.32	r<0	0.34	48 %
Winter wheat	USDA	Yes	0.64	0.65	0.35	0.33	0.28	50 %
	GGYD	Yes	0.55	0.91	0.26	0.00	0.00	10 %

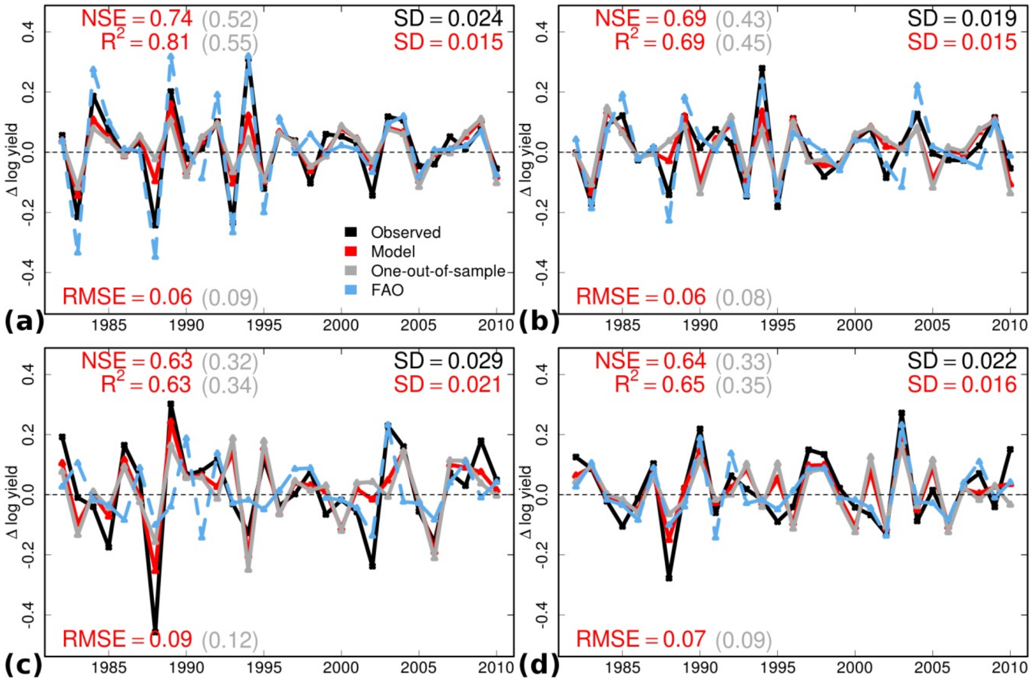

***Figure 2**: Observed and modeled time series of national US yield anomalies for maize (a), soybeans (b), spring wheat (c) and winter wheat (d). Black lines are anomalies of reported USDA yields, red lines are anomalies predicted by the model trained on the full data panel, gray lines are anomalies predicted from one-out-of-sample models, and blue dashed lines are FAO yield anomalies. Data points were 56,092, 38,373, 21,291 and 58,877 for maize, soybeans, spring and winter wheat, respectively. Numbers in plots are performance measures and standard deviation (SD); colors of numbers correspond to the respective anomaly series. Modelled and FAO yield anomalies were significantly ($p < 0.05$) correlated for maize (Pearson's r = 0.87), soybeans (0.69) and winter wheat (0.68), but not for spring wheat (0.13), since FAO yields combine spring and winter wheat.*

The model achieved at least two thirds of explained variance (R^2) and a robust (i.e. at least 25%) one-out-of-sample performance (R^2_{O1}) for all four crops with USDA data. Extremely low yields, like those occurring during the US heat and drought wave in 1988 for maize and wheat, were captured by the model, though not in full magnitude. For the two wheat types, yield loss quantities over the whole time series were comparable between model and observations, and for winter wheat also between one-out-of-sample model and observations. The set of three years of most negative yield anomalies (bottom decile) was equal for observed and modeled time series in 7 out of 12 cases. The observed top decile was captured in 8 out of 12 cases. For the one-out-of-sample predicted yields the correspondence for the bottom decile was less accurate with only 3 out of 12 cases. The direction of change and the sign of modeled anomalies matched with the input data for all crops, with only few exceptions.

The model performed differently for different crops, judged by R^2_{O1}. The regression method, variable set or difference method influenced model performance (SI Figure S6). Unweighted aggregation was better for maize, soybeans (except GGYD soybeans where R^2_{O1} was low) and spring wheat, but disfavored for winter wheat. Model performance differed between the two yield data sets. Although R^2 values were similar or higher for GGYD yields, R^2_{O1} values with GGYD data (Table 1, SI Figure S6) were lower in three of four cases. Differences between R^2 and R^2_{O1} were thus higher for GGYD yields. STSM models showed, on average over all crops and specifications, slightly higher R^2 and R^2_{O1} values than PDM models (SI Figure S6). R^2 and R^2_{O1} were correlated for USDA yields ($r = 0.97$, $p = 0$, $n = 24$), but not GGYD yields ($r = 0.29$, $p = 0.17$, $n = 24$). NSE and R^2 showed larger differences for GGYD than USDA yields. Thus the model's explanatory power was not an indicator for the model's projective power with GGYD yields. The out-of-temperature and out-of-precipitation performance (where six anomalies were omitted for training) was lower than the one-out-of-sample performance. All out-of-temperature values with USDA yields are, nevertheless, above 0.25, thus higher than expectable by chance (corresponding to $r = 0.5$). One-out-of-sample performance in the three warmest years is hardly different from modeled values. Out-of-precipitation values are above 0.25 only for wheat.

The explained variance varied spatially (Figure 3). There was a substantial fraction of grid cells where the model was able to capture yield variability to a large (green shades) or an intermediate extent (yellow shades). But there were also several regions where the model failed to capture variability (red shades). For all crops these were located in areas where yield variability was lower compared to other regions. In regions with substantial yield variation (coefficient of variation CV, defined as standard deviation over mean, is larger than 15%) the model achieved a higher R^2 more often (SI Figure S10; SI Table S2). There was a moderate fraction of grid cells (11-27%) that exhibited low yield variability and was not well explained by the model.

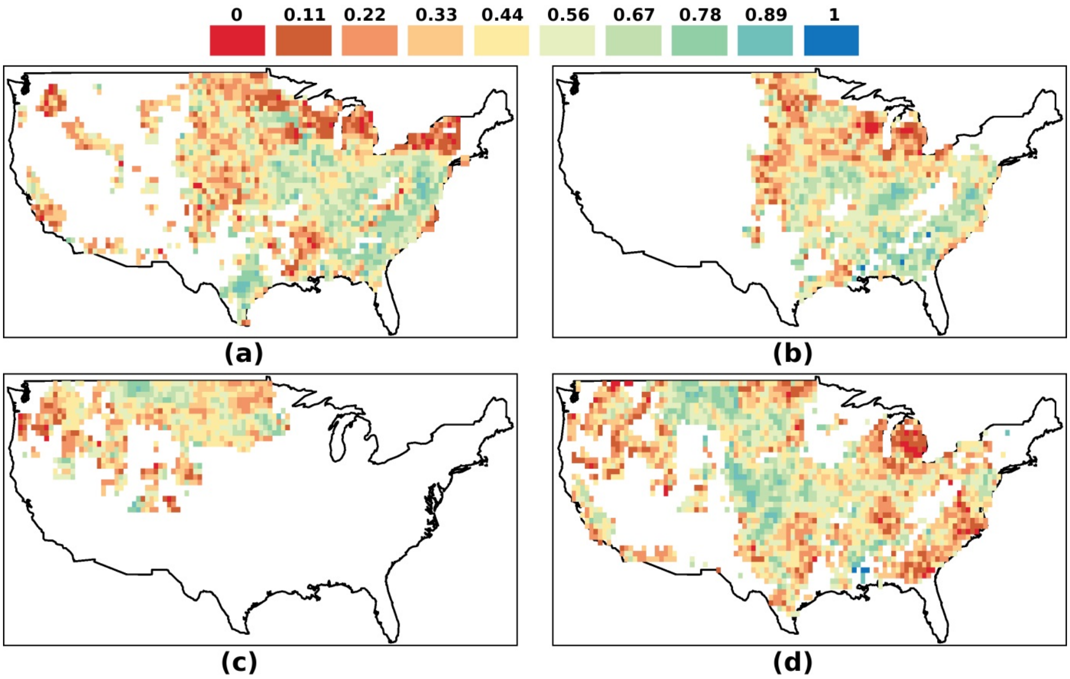

***Figure 3**: Explained variance of yield anomalies due to weather anomalies (R^2, color map on top) for maize (a), soybeans (b), spring wheat (c) and winter wheat (d) with USDA yields. White regions have no cropping area.*

Model coefficients indicated crop-specific patterns of weather influence. The influence of coefficients depended on the crop, but was independent from the estimation method (Figure 4). All STSM coefficient means except two were significantly different from 0 (t-test at 95% confidence level). For all crops a high PET in the reproductive period was clearly negative. Precipitation was positive for summer crops during the vegetative period and for soybeans and winter wheat also during the reproductive period. For spring wheat and maize too much precipitation during the reproductive period was negative. Normalized solar radiation was negative for maize and soybeans (vegetative period), but strongly positive for spring and winter wheat. Any day above 32°C was damaging for all crops (not significant for winter wheat), whereby maize was most affected. Days below -15°C or 0°C, respectively, were damaging for all crops, but did not occur during the spring wheat growing season. There was a marked difference of coefficient values between the two yield data sets (USDA, GGYD). This was the case for STSMs (SI Figure S7) and PDMs (SI Figure S8).

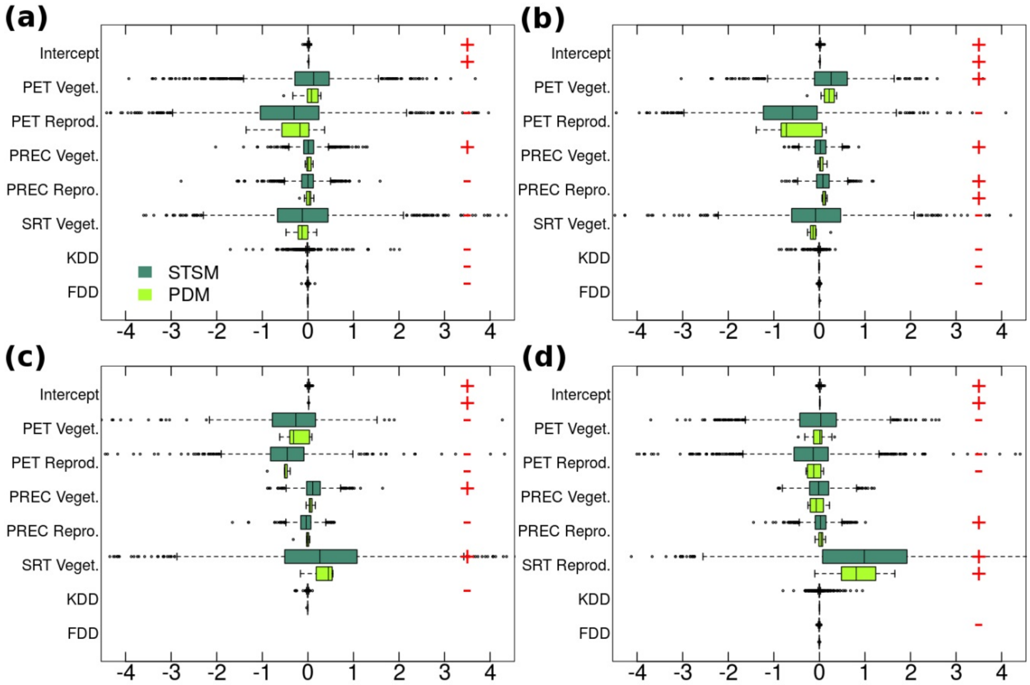

Figure 4*: Coefficient comparison for STSM and PDM model estimation for maize (a), soybeans (b), spring wheat (c) and winter wheat (d) with USDA yields. Blue boxes show coefficients with STSM estimation (estimated for each grid cell), while green boxes show PDM coefficients (estimated for each climate region). The band inside each box is the median, while boxes represent 25% and 75% quantiles. Whiskers are defined as the maximum and minimum as long as both values are within the 1.5 interquartile range from the median. Otherwise the last points in this range are shown with whiskers and outliers are depicted as points. Red +/- symbols indicate a mean significantly larger/lower than 0 (t-test at 95% confidence level).*

Coefficients varied between climate regions (Figure 5). A high PET during the vegetative season was positive for maize yield in the northern climate zones, but negative in the south. Vegetative PET was positive everywhere for soybeans. For spring wheat a high PET was negative everywhere except the northwest. For winter wheat a high PET during the reproductive season was positive only in the northeast, but negative elsewhere. The effect of precipitation did not show pronounced regional diversity: it was positive in most regions for all crops, with few exceptions. Elevated SRT during the vegetative period had a positive effect on maize yields in mid and western states, but not elsewhere. Enhanced SRT was negative for soybeans in all regions. For spring wheat, by contrast, higher SRT was positive everywhere except the northwest. For winter wheat more SRT had positive effects during the reproductive period in almost the whole US, with a positive gradient to the southeast. Days above 32°C were harmful everywhere for maize, spring and winter wheat (-2 to -4% yield loss for each day).

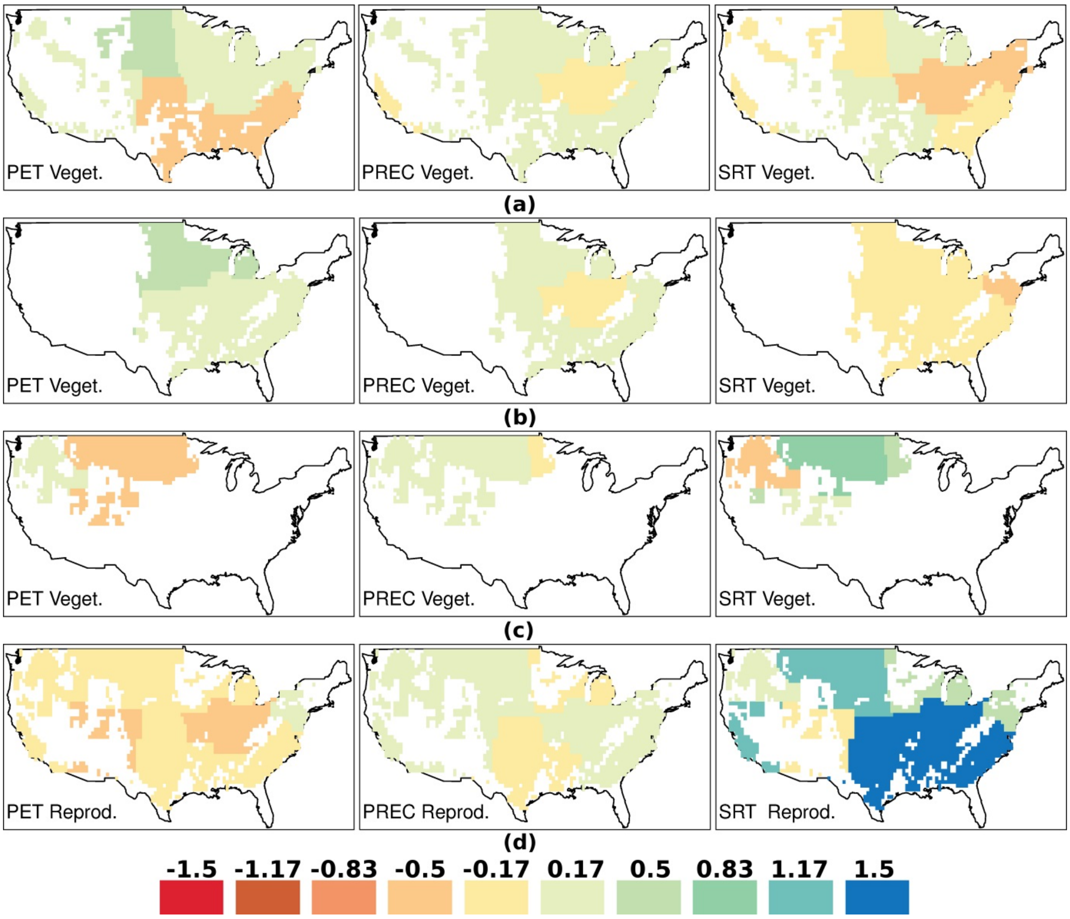

***Figure 5**: Estimated coefficients for USDA yields. Rows are maize (a), soybeans (b), spring wheat (c) and winter wheat (d). Coefficients were estimated with STSM regression and aggregated from grid cells to climate regions. From left to right the coefficients are PET in vegetative (maize, soybeans, spring wheat) or reproductive (winter wheat) season, precipitation and SRT in the same seasons, respectively. Color map is shown at bottom.*

A mapping sensitivity test, where climate, land-use and growing seasons were interpolated from grid cells to counties rather than yields from counties to grid cells, showed similar or slightly higher R^2 (0.82, 0.74, 0.65 and 0.68 for maize, soybeans, spring and winter wheat, respectively) and R^2_{O1} values (0.61, 0.55, 0.34 and 0.30). We kept the mapping of yields to grid cells, though, to maintain a common framework for both yield data sets.

Results for global main producers

The model explains more than two thirds of yield variance in main producer countries. The robust out-of-sample performance in the US supported an extension of the evaluation to other main producers (SI Table S3; Figure 1). Only GGYD yields could be used as generally available source here. Nationally aggregated GGYD yield anomalies mostly corresponded well with FAO yield anomalies (SI Figure S12), motivating the usage of this data set. The performance (R^2 and R^2_{O1}) for all crops is displayed in Figure 6. The explained variance among main producers, weighted by total production, was 84%, 72%, 71% and 71% for maize, soybeans, spring and winter wheat, respectively. The weighted average one-out-of-sample performance was 42%, 22%, 33% and 15%. The cumulative production share (within the main producers) of nations which achieved an R^2_{O1} of at least 25% is 64%, 18%, 68% and 30% for maize, soybeans, spring and winter wheat, respectively. Analyses with PDM estimation led to similar, though slighty lower performances (SI Figure S14). Calculating aggregated model performance as average performance over all grid cells in a country, rather than by correlating previously aggregated yield time series, resulted in lower model performances: mean R^2 [R^2_{O1}] STSM values over countries were 0.47 [0.18], 0.44 [0.15], 0.48 [0.19] and 0.36 [0.10] for maize, soybeans, spring and winter wheat. This aggregation effect, as discussed in Gornott and Wechsung (2016) for Germany, was thus confirmed globally.

Yield time series for selected main producers can be found in the supplement (SI Figure S13). Mean performance was best for maize (highest R^2 and R^2_{O1}). While R^2 was similarly high for soybeans, the R^2_{O1} was rather low (22%). For winter and spring wheat the model achieved equal mean R^2, while mean R^2_{O1} was substantially higher for spring wheat. There was no obvious influence of harvested area, length of yield time series, share of rainfed agriculture, mean yield level or standard deviation on model performance. Countries where GGYD yields were constructed from subnational data (Table S1 in Iizumi *et al.* (2013b)) tended to have a larger R^2_{O1}, but not significantly. There are some notable discrepancies between R^2 and R^2_{O1}, especially for winter wheat: for example in India or Egypt an R^2 of 0.93 and 0.73, respectively, was accompanied by an R^2_{O1} of 0.04 and 0.03. In both cases, this discrepancy is due to extreme yield values captured by the model, but not the one-out-of-sample model (data not shown). If these extremes are removed, R^2_{O1} increases to 0.16 and 0.22, respectively. Differences between R^2 and R^2_{O1} are generally due to an out-of-sample time series which is less variable and captures fewer extreme values than the modeled time series.

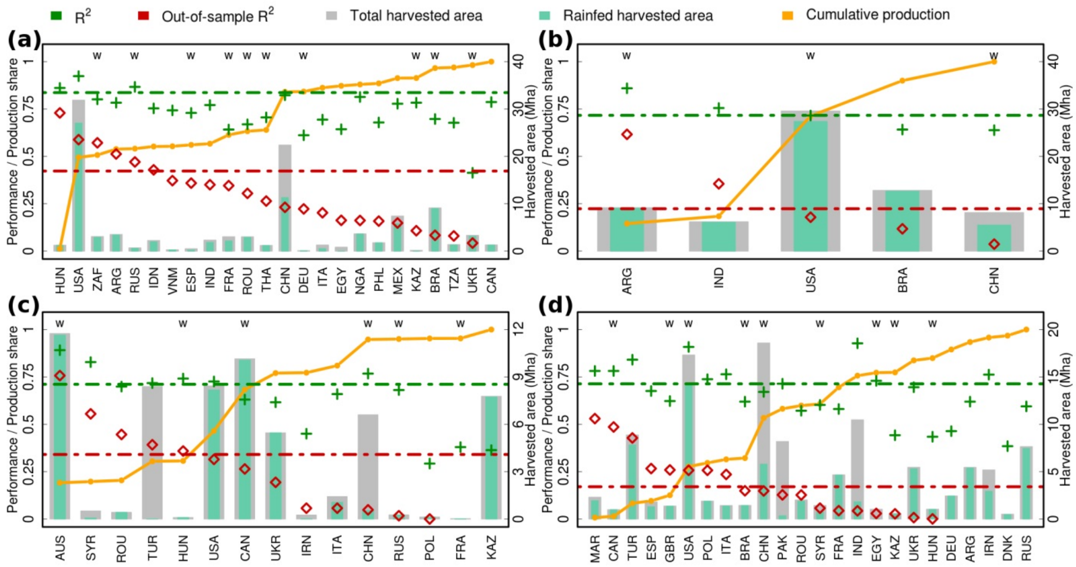

Figure 6: Performance of STSM models in main producing countries for maize (panel a), soybeans (b), spring wheat (c) and winter wheat (d). Countries are ordered by descending R^2_{O1}; three-letter codes are provided in SI Table S3. Green crosses mark R^2 and red diamonds R^2_{O1} values (left y axis). The mean R^2 and R^2_{O1} over all main producers, weighted by production, are indicated with dashed green and red lines, respectively. A "w" above countries indicates that the displayed R^2_{O1} value is achieved when including land-use weighting. Gray and blue bars denote total and rainfed harvested area in Mha, respectively (right y axis). The orange line denotes cumulative production share among main producers (left y axis).

Yield data quality influences the detection of weather influences. There was a marked difference in model performance when using either reported sub-national yield data or gridded yield data derived from remote sensing. R^2_{O1} values for USDA data were 55%, 45%, 34% and 35% for maize, soybeans, spring and winter wheat, respectively, while for GGYD data these were 59%, 18%, 32% and 26%, thus lower except for maize (Table 1). This difference was also visible for Germany, Russia, Burkina Faso, Tanzania and Brazil (SI Table S4).

The average explained variance over all main producing countries and crops was 41.8% with GGYD yields. This was slightly higher than the 32-39% which have been found by Ray *et al.* (2015) with reported data. For maize the average R^2 was 44% with our model, compared to

39% in Ray *et al.*, and for soybeans it was 42%, compared to approx. 35%. For wheat (average over spring and winter) it was 42% with our model, compared to 35%.

Yield anomalies are forecasted with high accuracy within the growing season in several countries. The model was used for a simple forecasting of yields up to two months before harvest. The results for countries with reported yields are shown in Figure 7, for all main producers using GGYD yields in SI Figure S15. In all but five (out of 14) cases the one-out-of-sample performance is equal or even higher than the standard model when omitting the last month of the reproductive season for training and prediction. In seven cases this holds also when omitting the last two months. In ten cases yield anomalies can be predicted better than by chance ($R^2_{O1} > 0.25$) two months before harvest, and in six cases this prediction accuracy is more than 50%. When using GGYD yield data, 25 of 63 cases can be predicted with at least 25% accuracy two months before harvest (representing 4-86% of global production depending on the crop), and in six cases with 50% accuracy (representing 0-51% of global production).

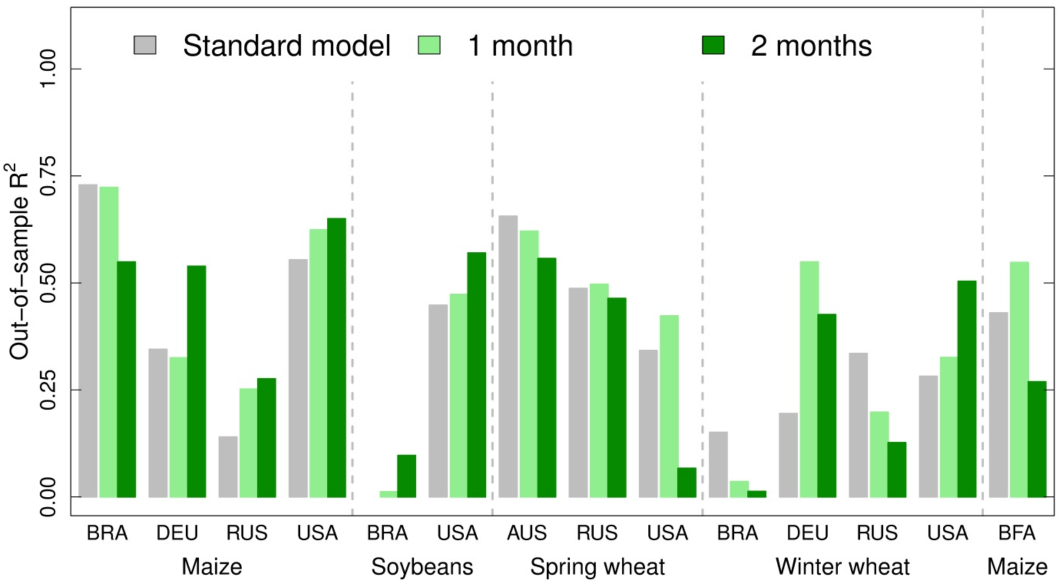

***Figure** 7: Capacity of the model for yield forecasting within the growing season, using only reported yield data. The one-out-of-sample performance R^2_{O1} is shown. Gray bars are the standard model with full growing season used for training and prediction. Green and black bars show performance when withholding one or two months, respectively, for training the model and predicting yield anomalies out of sample. Burkina Faso (BFA) is not a main producer and therefore plotted off set.*

Mean warming suggests negative yield effects. When increasing temperatures by 0.9 or 1.4 °C above the 1980-2010 average, yields are predicted to lose 3-18% (excluding Australian wheat and Brazilian soybeans) in comparison to reported yield data (Table 2). Results for Russia had high uncertainties due to large $RMSE_{O1}$ values and standard deviations. Projections based on GGYD yields were not performed due to low R^2_{OOT} scores (Table 1).

***Table 2**: Yield effects (as fraction of average historic yields) of artificial temperature increases, using only reported yield data. Fractions were normalized with T+0 offset. Values in brackets are uncertainty measures u (+/-) of the fraction according to equation 5.*

Crop	Country	T +0.9 °C	T +1.4 °C
Maize	USA	0.96 (0.07)	0.95 (0.07)
	Russia	0.88 (0.87)	0.85 (0.86)
	Brazil	0.97 (0.19)	0.95 (0.20)
	Germany	0.96 (0.09)	0.94 (0.09)
	Burkina Faso	0.95 (1.00)	0.94 (1.00)
Soybeans	USA	0.97 (0.16)	0.96 (0.17)
	Brazil	1.00 (0.12)	1.00 (0.12)
Spring wheat	USA	0.95 (0.16)	0.92 (0.17)
	Australia	1.05 (0.71)	1.07 (0.74)
	Russia	0.89 (0.77)	0.84 (0.83)
Winter wheat	USA	0.97 (0.07)	0.95 (0.07)
	Russia	0.88 (0.72)	0.82 (0.78)
	Germany	0.95 (0.06)	0.92 (0.07)
	Brazil	0.89 (0.32)	0.85 (0.36)

DISCUSSION

We have applied a semi-empirical regression model to estimate weather influences on yields of maize, soybeans, spring and winter wheat. The model achieves good performance in explaining and predicting inter-annual yield variation in the US. For all main producer countries a high average explanatory power but varying out-of-sample prediction capacity is attained. The model shows medium to high accuracy for yield anomaly forecasts during the growing season up to two months before harvest. An application of the model with artificially increased temperatures suggests negative effects of moderate warming on crop yields.

Modeling yield anomalies in the US

The fraction of explained yield variation was at least two thirds and the one-out-of-sample yield prediction accuracy achieved 34-55%. The model also achieved a quantitative reproduction of negative yield anomalies in most cases, which is of particular importance when studying non-linear economic responses. When validating the model in the warmest or driest years its out-of-sample capacity is better than 25% in six of eight cases (Table 1, USDA).

Explanation (R^2) and projection (R^2_{O1}) capacity were strongly different (up to 0.65) in some cases, and more so for GGYD yields (SI Figure S6), underlining that both model fit and out-of-sample performance should be considered when evaluating the quality of a model (Holzkämper *et al.*, 2015, Landau *et al.*, 2000, Refsgaard *et al.*, 2013). Differences between NSE and R^2 values could be due to an over-proportional influence of outlier values or scale effects on the NSE.

The different out-of-sample performance of the model with USDA and GGYD yield data, in particular for soybeans and winter wheat, suggests several uncertainties of the gridded yield data. First, the combination of reported yields with remote sensing data and growing season modeling might not be apt for winter crops as these are more easily mixed with other vegetation. Second, the time series of the GGYD data is shorter by six years, leaving less data for out-of-sample estimations. Yet a regression with USDA yields in the shorter GGYD time frame produced similar results as with the full range (data not shown), thus the shorter time series alone is unlikely to explain different performances. Third, the equal or higher average R^2 with GGYD yield data (SI Figure S6) could possibly result from an implicit consideration of weather influences in the GGYD data set or the fitting of the model to more extreme values which arose in the GGYD construction but are not necessarily caused by weather. A misestimation of the true weather influence with our model would ensue. FAO yields, which are used in GGYD construction to calibrate remote sensing data, are often combined from reported and estimated data, adding a further layer of uncertainty. Fourth, yield variability from small plot sizes, in particular in developing countries, could be flattened at the coarse aggregate scale and thus blur weather influences. Fifth, GGYD yields showed lower CVs than USDA yields (except spring wheat, SI Table S2). This may explain the larger differences between R^2 and R^2_{O1} for GGYD yields, as low CVs together with shorter time series can lead to high correlations, but instable models i.e. a low R^2_{O1}. Similar differences in model performance between observed and remote sensing-derived yields in other nations (SI Table S4) further support our conclusions.

The geographical variation of model performance could have several causes. Different management techniques eliminate different shares of weather influence on crop yield. In particular irrigation, which is more prominent in the Western US (Schlenker & Roberts, 2009), marginalizes the effect of precipitation and also temperature (Lobell & Bonfils, 2008, Schauberger *et al.*, 2017). This is underlined by a lower model performance in this region (Figure 3). Thus, a low explanatory power might reflect a limited influence of weather on yields, as our model only detects weather impacts. Other reasons could include unconsidered, indirect weather influences (e.g. pests or diseases), errors in observations or aggregation effects. This may also explain the substantial share of grid cells with high yield variability but low explanatory power (SI Table S2). Low yield variability is difficult for any model to capture. Combined analysis of yield variation and model explanatory power reveals that areas with low yield variability are more likely to have a lower R^2 (SI Table S2, SI Figure S10). Areas with a high USDA yield CV, by contrast, have equal shares of high and low explained variance. Uncertainties introduced by interpolating yield or weather statistics could destroy their associations (Hansen & Jones, 2000). A comparison of our results using GGYD data to the global study by Ray *et al.* (2015), using reported data, revealed a similar or larger share of grid cells with substantial yield variability but unsatisfactory explained variance ($R^2 < 0.45$) in Ray *et al.* Our results suggest, again, that yield variability in many agricultural areas is influenced by more factors than only weather. These could include changing land-use patterns (Olmstead & Rhode, 2011), economic influences like fertilizer usage or stressors like ozone or pests.

The estimated coefficients and their geographical distributions agree with expectations. Maize reacted negatively to a high PET in the reproductive season and to very hot days (KDD) in particular in warmer regions – which agrees with previous findings (Lobell *et al.*, 2013, Schlenker & Roberts, 2009). This is contrary to expectations that C_4 crops would not experience much damage from mild heat (Sage & Kubien, 2007), but is likely due to water stress prior to direct heat damages (Schauberger *et al.*, 2017). This effect also explains the higher model performance for maize and soybeans in the South, where water stress is more dominant. PET in the vegetative season and solar radiation affected maize positively only in cooler regions, confirming previous studies (Long *et al.*, 2006, Rötter & Van de Geijn, 1999). Precipitation effects seem limited, though vegetative precipitation was usually positive. This conforms with a larger water demand of maize during the vegetative season (Hlavinka *et al.*, 2009). The relatively low precipitation coefficient values, despite its prominent importance (Barnabas *et al.*, 2008, Troy *et al.*, 2015), are due to comparably high and strongly varying input values (Gornott & Wechsung, 2016, Lobell *et al.*, 2013).
Differences in C_3 (soybeans, wheat) and C_4 (maize) photosynthesis efficiencies (Long *et al.*, 2006, Rötter & Van de Geijn, 1999) are reflected in a lower positive effect of SRT for maize. KDDs were less negative for winter wheat than for maize, since these hardly occur during the growing season – winter wheat is usually harvested before heat waves build up. A higher PET in the reproductive cycle was more detrimental than a higher PET in the vegetative cycle of either winter wheat or maize due to a more developed canopy. This also applies to precipitation effect differences between the reproductive winter wheat and the vegetative maize cycle. The model performance was low for all crops in the Northwest, and only slightly higher in the East North Central region. These regions seem more stable against weather fluctuations.

Six independent statistical tests indicated that our OLS estimation approach is applicable. Quadratic variables would not improve the model fit although this technique is often used to capture non-linear influences (Lobell *et al.*, 2011, Ray *et al.*, 2015). Autocorrelation occurring in many grid cells (SI Figure S9) points to periodically occurring yield variability, which might lead to an underestimation of standard errors with OLS. But this autocorrelation is due to autocorrelation in the raw yield data (55%, 32%, 31% and 37% of grid cells for maize, soybeans, spring and winter wheat, respectively, at 95% confidence level with a Ljung-Box test) and the first difference approach which produces correlated yield differences. Therefore we assume it as unproblematic for our analysis. The nationally aggregated time series was weakly autocorrelated for soybeans and winter wheat and not autocorrelated for maize and spring wheat.

When calculating yield variability on spatially aggregated level, a land-use weighting is usually applied to capture spatially divergent contributions to agricultural production. But model performance was better with unweighted yields except for winter wheat, whose growing area is less concentrated (SI Figure S3). Land-use patterns can be considered as an indirect function of climate since crops more favored by a certain climate also tend to have more area share. Thus there is an implicit inclusion of land-use patterns in the estimated coefficients, which makes the weighting negligible when inspecting aggregated yield variability. The differences are not substantial in all cases, which further suggests that land-use weighting can be omitted. This is beneficial for model generalization since weighting is another level of uncertainty (Cohn *et al.*, 2016, Porwollik *et al.*, 2016).

The model only used monthly aggregated weather data as input. This is an advantage over models requiring daily weather input since monthly aggregates are the preferred output from climate models (Taylor *et al.*, 2012) and are also less sensitive to outliers. The yield-anomaly approach of our model additionally eliminates any time-dependent systematic bias. It is therefore particularly apt for usage with data from climate models, which often require a bias correction before impact assessments (Hempel *et al.*, 2013).

Application to main producers

The generally good correlation between GGYD and FAO yield anomalies (SI Figure S12) allows us to interpret aggregated production from GGYD yields and MIRCA2000 areas as representative for main producing countries. The average R^2_{O1} was at least one third for maize and spring wheat. For soybeans and winter wheat average R^2_{O1} was low, which is likely due to shortcomings of GGYD data with these crops (see above and below). This is supported by the increased performance of the model when using reported yield data (SI Table S4).

More than half of the global maize and spring wheat production anomalies could be well explained by our model (R^2_{O1} at least 25%). This enables the usage of our model in global economic assessments. We assume this share to rise with more reported yield data.
Countries with a high predictive capacity of the model (R^2_{O1} above or around 50%) all have water-dominated yield variability, i.e. the majority of cultivated area being rainfed and a rather high alternation between deficient and sufficient precipitation. This suggests that the model particularly captures water-limiting signals, though this may be questioned by the low R^2_{OOP} with GGYD yields (Table 1). Wheat grown in Morocco and Turkey was classified as winter wheat due to its relatively long growing season (7-11 months) over the local winter, but is different from "classical" winter wheat grown in cooler nations where the crop experiences a vegetative pause over the winter. This could bias results towards lower R^2 values. The performance of our semi-empirical model, when run with reported yield data, was equal or superior to several previously applied statistical approaches (Iizumi *et al.*, 2013a, Lobell & Field, 2007, Ray *et al.*, 2015, Urban *et al.*, 2012).

We analyzed GGYD yields as an alternative to reported yields in areas where such data are currently not available. But the model-based nature of the data set could introduce a bias to our results. The robust performance of the semi-empirical model in the US, Germany, Russia, Burkina Faso, Tanzania and Brazil allows its usage for identifying cases where GGYD yields presumably suffer from a construction bias. We speculate that an existing weather influence on crops could be blurred by GGYD construction steps and is therefore less detectable with our (or any weather-driven) model. R^2 and R^2_{O1} values are then further apart, for example due to GGYD-processing induced yield extremes that are uncoupled from weather influences. The less convincing results for soybeans and winter wheat match with the evaluation by Iizumi *et al.* (2013b) suggesting that GGYD data likely requires improvement for both crops. A remaining concern is whether estimating a statistical model from a data set (GGYD) and then using the same model to evaluate these data may confound conclusions. But two additional analyses confirm our assumption that estimation problems occur more likely when GGYD yields are involved. First, the out-of-sample performance of models trained on reported yields is clearly superior to models trained on GGYD yields (SI Table S4). Second, a cross-comparison of model-predicted yields with reported FAO data, but where the model has been estimated with GGYD data (SI Figure S14), shows that there are discrepancies for all crops. Differences between predicted yields and FAO are usually smaller when using reported yields for training the model (dashed blue lines in Figure 2). Nevertheless we esteem the unique ability of GGYD yields to cover all regions of the globe where subnational yield data are otherwise difficult to obtain. Usage of latest satellite data with more sophisticated land-use separation methods may reduce counter-factual error sources and thus increase the reliability of satellite-derived yield statistics (Iizumi & Ramankutty, 2016).

Yield forecasting and warming experiment

The model concept allows for a simple extension towards forecasting of yields few months before harvest. This study presents a first example application in this direction. The forecasting is robust (R^2_{O1} > 50%) up to two months before harvest in several major producing countries, but requires improvement in others, in particular for soybeans and winter wheat. The performance is thus comparable to previous approaches (Bolton & Friedl, 2013, Johnson, 2014, Sakamoto *et al.*, 2014), but has been done here without any particular adaptation to country-specific conditions or model formulation. In several cases the reduced growing season leads to higher R^2_{O1} values than the full season. This could stem from three reasons. First, crop climatic requirements can be different in grain filling and maturity phase (Barnabas *et al.*, 2008), which are not distinguished in our reproductive season and could lead to meaningless coefficients in the default model. Second, the growing season dates in MIRCA2000 could be wrong, leading to an improvement when omitting a too long part. Third, the vegetative and reproductive season split could be misplaced. These reasons will have to be investigated in further studies. Again, the importance of high-quality input yield data for model training is highlighted: only then reliable within-season forecasts are possible, as evidenced by the lower performance with GGYD yields.
The forecasting scheme could be modified in two directions. Both require near-term monthly weather forecasts published, for example, by the NOAA (NOAA Climate Forecast, 2017). First, the full growing season can be used for training. In the season where yields should be predicted before harvest the missing part of the weather information is supplied by a near-term forecast. Second, both approaches can be combined: a reduced growing season, e.g. withholding the last two months of the season, is used for training. Yield predictions are then calculated for three or more months before harvest by supplying the missing weather information up to two months before harvest with near-term weather forecasts.

Predicting yields with counter-factual temperature increases is another model application case. The approach neglects CO_2 trends, variation of cofactors like precipitation and comes with high uncertainties (out-of-temperature performances in Table 1 and the *u* measure according to equation 5 provide a first, maybe too high estimate), which might mask effects. This could change if real climate scenarios were used including drifts in temperature extremes and precipitation. But impacts seem plausible in direction and magnitude compared to previous studies (Challinor *et al.*, 2014, Giannakopoulos *et al.*, 2009, Schleussner *et al.*, 2016). The low R^2_{OOT} performance for GGYD yields underlines the importance of high-quality yield data when projecting future yields. The average decline in wheat yields, when averaged over spring and winter wheat at 0.9°C warming (Table 2), is 6% – in agreement with the results by Liu *et al.* (2016). Thus the semi-empirical model described here can be considered a fourth method next to the three methods considered therein.

The model scheme presented in this study is an open concept that can be extended to incorporate further weather or economic factors. The prediction of yields within the growing season is highly sought after for timely adaptation measures in management, storage or marketing. Our model will be further developed in this direction. The differential performance between observed and remote-sensing based yield data calls for better and publicly available yield data from statistical offices in all countries. These can aid in planning adaptation or evaluating, for example, agricultural micro-insurance schemes.

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5.2 Supplementary Information

The supplementary information is printed in scaled form since its original version is also available with the online version of the article.

Supplementary Information to "Global evaluation of a semi-empirical model for yield anomalies and application to within-season yield forecasting"

B. Schauberger et al.

1. US climate regions, growing seasons, land-use patterns and reported yields used in this analysis

A map of the nine US climate regions used in this study is shown in Figure S1. Their definition is based on Karl and Koss (1984). The average climate during the average maize growing season according to MIRCA2000 (Portmann *et al.*, 2010) is shown in Figure S2. Land use fractions according to MIRCA2000 are shown in Figure S3. The distribution of growing seasons according to MIRCA2000 is shown in Figure S4. For maize and soybeans calculated vegetative months of the average growing season in the US are April to June; calculated reproductive months are July to October. For spring wheat the split is May to June (vegetative) and July to August (reproductive). For winter wheat the vegetative part is October to April and the reproductive part May to July. The first months of the calculated reproductive seasons correspond with observed anthesis dates by the USDA[1]. Nationally aggregated yield time series, together with two anomaly calculation methods, are shown in Figure S5. The equations used for aggregating grid cell time series to national averages are listed in supplementary equations SE1 and SE2. The equations used for defining PHUs and the ensuing split between vegetative and reproductive parts of the growing season are provided in equations SE4 and SE5 (section 2).

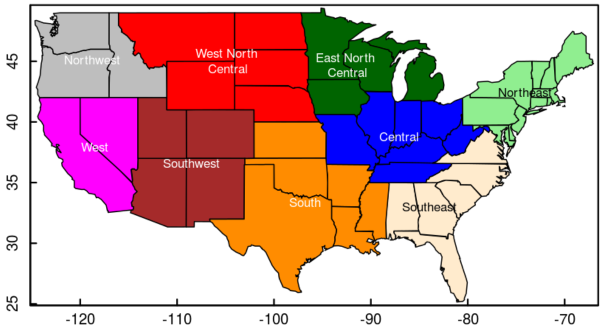


Figure S1*: The nine climate regions of the US as applied in this study.*

[1] http://www.usda.gov/oce/weather/pubs/Other/MWCACP/MajorWorldCropAreas.pdf ; accessed on July 20, 2016

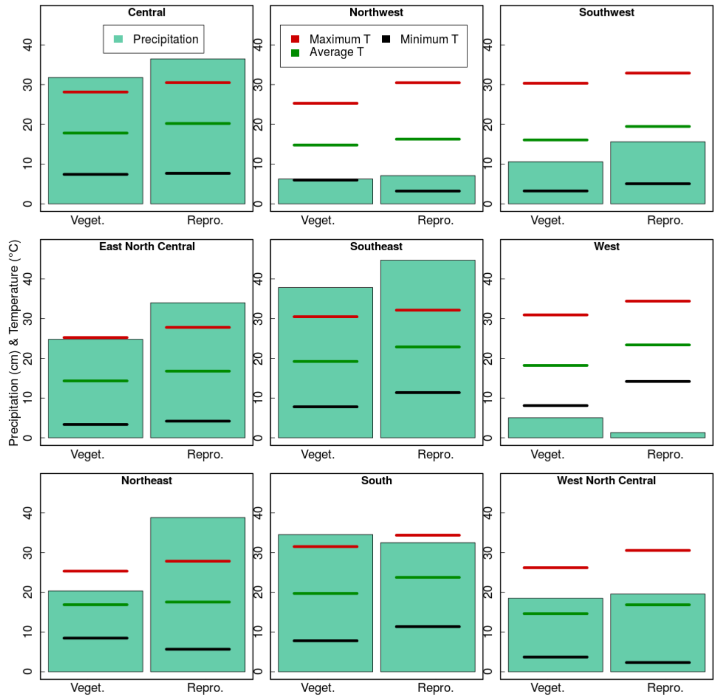
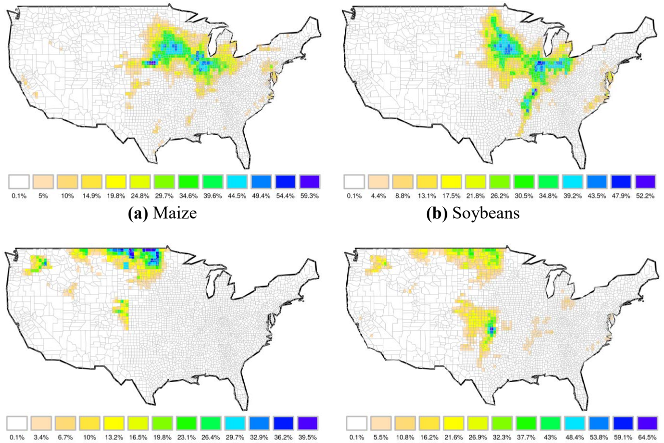


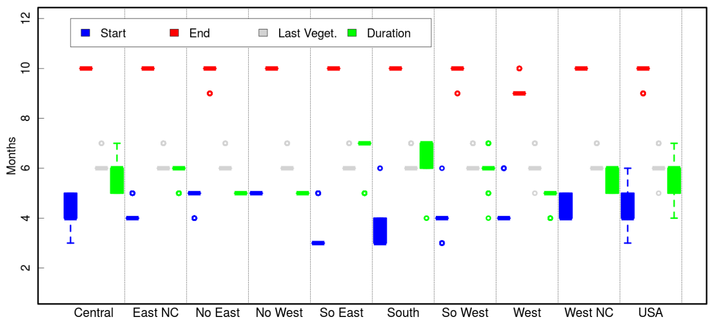
Figure S2*: Climate diagrams for the nine US climate regions during their maize growing season. Precipitation (in cm) and temperatures (in °C with minimum as blue, mean as green and maximum as red horizontal lines) are split into a vegetative and a reproductive part. Averages are calculated over space and time; the temperature extrema are averages over the individual grid cell extrema. The maize growing season according to MIRCA2000 (Portmann et al., 2010) can vary between regions (Figure S4).*



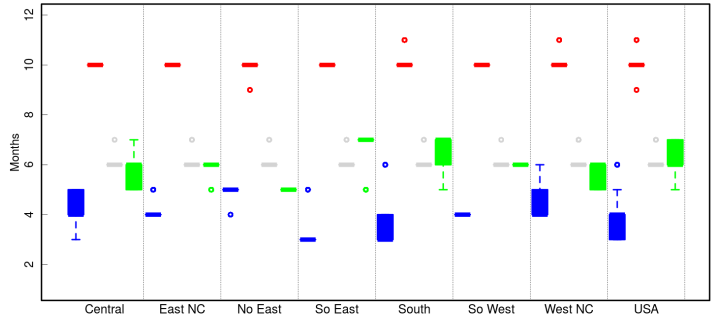
(a) Maize (b) Soybeans

(c) Spring wheat (d) Winter wheat

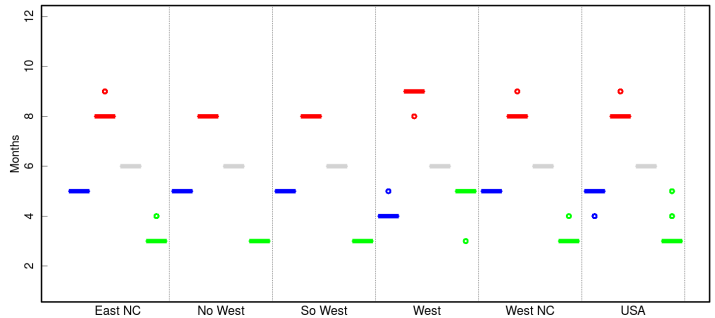
***Figure S3**: Land use fractions as percent of grid cell area for maize (a), soybeans (b), spring wheat (c) and winter wheat (d) according to MIRCA2000 (Portmann et al., 2010). County boundaries are drawn in grey. Color scales diverge between land use maps.*



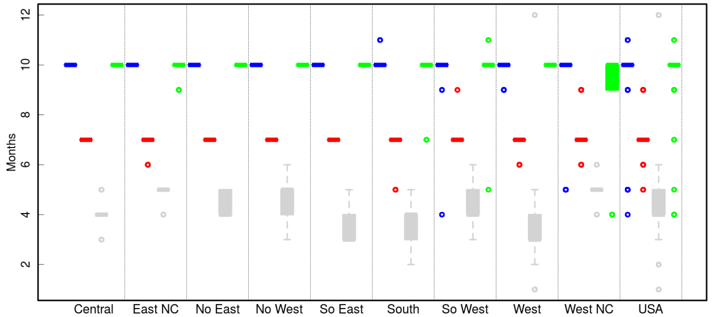
(a) Maize



(b) Soybeans



(c) Spring wheat



(d) Winter wheat

***Figure S4**: Distribution of growing season start and end months (blue and red boxes, respectively), the last month of the vegetative growing season as defined by the 50% PHU threshold (see equations SE4 and SE5; grey boxes) and the duration of the growing season in months (green boxes). Several boxes are condensed to lines since there is no variation in the data. There is, in general, only little variation of growing seasons across the US according to MIRCA2000.*

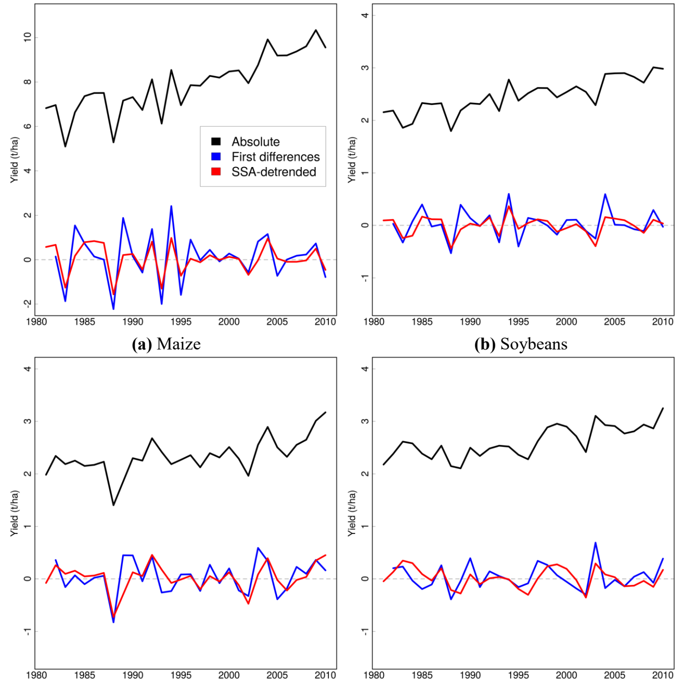
The equation used for aggregating time series from grid cells to climate region or country level is provided in equation SE1.

$$\bar{y} = \frac{\sum_i l_i * a_i * y_i}{\sum_i l_i * a_i} \qquad \text{(eq. SE1)}$$

where y_i is yield anomaly in grid cell i, a_i is area of grid cell i, l_i is fraction of total land-use for the specific crop in grid cell i and $\bar{y}$ is the averaged yield anomaly over all grid cells in the aggregation region. If aggregation is weighted, l_i is taken from MIRCA2000 and a_i is calculated by equation SE2. If aggregtion is unweighted, both l_i and a_i are set to 1, resulting in the standard average.

$$a_i = {r_E}^2 * (\lambda_{i,2} - \lambda_{i,1}) * (\sin\varphi_{i,2} - \sin\varphi_{i,1}) \qquad \text{(eq. SE2)}$$

where r_E is earth radius (6,371 km), λ and φ are longitude and latitude boundaries of the grid cell (in radians).



(a) Maize **(b)** Soybeans **(c)** Spring wheat **(d)** Winter wheat

***Figure S5**: Time series of yields for four staple US crops. Black lines are nationally aggregated yields, calculated from grid cells with land-use fraction for the respective crop larger than 0 and weighing by these land-use fractions. Blue and red lines, respectively, show yield anomalies calculated from these nationally aggregated yields by calculating either first differences between adjacent years (blue) or by subtracting a parameter-free Singular Spectrum Analysis trend (red).*

2. Full regression equation

The full regression equation is provided in supplementary equation SE3. This 'standard' regression can be modified by three switches (for sensitivity analyses): estimation method, included variables and anomaly calculation (Table S1). All combinations between all values (12 in total) are evaluated for each crop, yield data set and aggregation weighting combination (16 in total). This results in a total of 12 * 16 = 192 regressions for the US. The equations used to calculate phenological heat units and to deduce the transition month between vegetative and reproductive season are given in equations SE4 and SE5.

Equation SE3 provides the fully specified 'standard' STSM regression formula for summer crops (i.e. with only the vegetative part of the temperature-corrected solar radiation). The equation contains eight coefficients including the intercept to be estimated ($\beta_{0..7}$) for each grid cell. For PDMs fewer coefficients are estimated: there is only one set for $\beta_{0..7}$ per aggregation region, but fixed effects allow for grid cell-specific intercepts.

$$\log Y_t{}' = \log \beta_0 + \beta_1 \log PET_{veg,t}{}' + \beta_2 \log PET'_{rep,t} + \beta_3 \log PR'_{veg,t} + \beta_4 \log PR'_{rep,t} + \beta_5 \log Rs'_{veg,t} + \beta_6 \log KDD_t{}' + \beta_7 \log FDD_t{}' + \log u'_t$$
(eq. SE3)

Variables are yield (*Y*), potential evapotranspiration (*PET*) during the vegetative (*veg*) and reproductive (*rep*) growing season parts, precipitation (*PR*) split into its vegetative and reproductive parts, temperature-corrected solar radiation (*SRT*) in the vegetative part of the growing season, killing and freezing degree days (*KDD*, *FDD*) over the whole growing season. The prime (′) behind each variable denotes yield anomalies. All variables are given for years (*t*) 1981 to 2010, starting one year later than data is available due to the first differences approach (two years later for winter wheat).

Table S1: *Possible values for the three regression switches. All 12 combinations of the three specifiers are allowed.*

Method	Variable set	Anomaly calculation
Separate Time Series Model ("STSM")	SRT (temperature-corrected solar radiation)	First differences ('first')
Panel Data Model ("PDM")	KDD-SRT (killing and freezing degree days plus SRT)	Difference to a singular spectrum analysis trend ('ssa')
	KDD-rad (KDD and FDD plus uncorrected solar radiation)	

Phenological heat units (PHU) above a base temperature over the growing season are calculated by equation SE4:

$$PHU_d = \sum_{i=1}^{d} \max(T_i - T^{base}; 0) \qquad \text{(eq. SE4)}$$

where *d* is a day during the growing season (starting with 1), T_i is the temperature at day *i* and T^{base} is a crop-specific base temperature (8°C for maize and soybeans and 0°C for spring and winter wheat). PHUs for a month are calculated by multiplying the PHU calculated from the monthly mean temperature by the number of days in this month.

The first month of the reproductive season for each grid cell and crop is calculated by equation SE5:

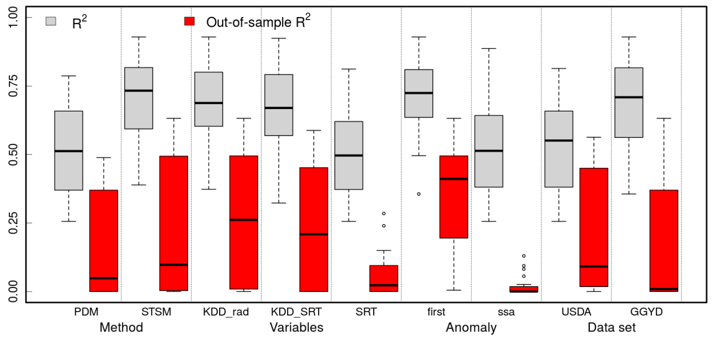
$$FRM = min_m(PHU_m \geq 0.5 * PHU_{max}) \qquad \text{(eq. SE5)}$$

where *FRM* is "first reproductive month", *m* is a month in the growing season, PHU_m is the PHU for this month according to equation SE4 and PHU_{max} is the total PHU achieved over the growing season.

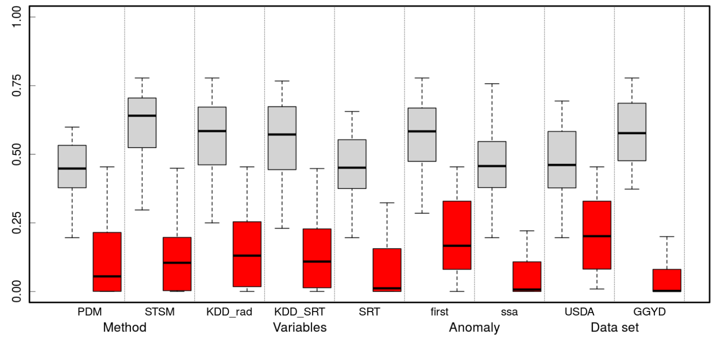
3. Model evaluation in the US

The performance ranges of different regression setups in the US are summarized in Figure S6. For each crop the distributions of R^2 and R^2_{O1} across several model specifications are provided. Abbreviations are as follows. Regression method is either PDM (Panel Data Model) or STSM (Separate Time Series Model). Variables are either “KDD_rad” (uncorrected radiation instead of SRT, with KDD=Killing Degree Days and FDD=Freezing Degree Days variables), “KDD_SRT” (temperature-corrected radiation and KDD/FDD variables) or “SRT” (only temperature-corrected radiation, but without KDD/FDD). Yield anomaly calculation is done by either first differences (“first”) or with a parameter-free trend estimated with Singular Spectrum Analysis (“ssa”). The data set can be either “USDA” (reported yield data provided by the USDA) or “GGYD” (global yield data derived from remote sensing and (sub)national yield statistics).

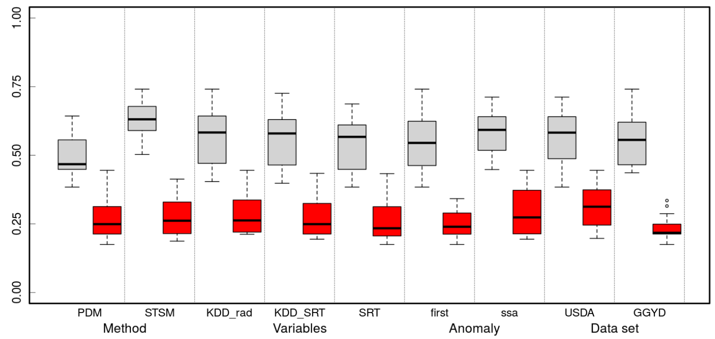
There is a strong discrepancy between regression coefficients estimated from either reported or GGYD yield data, for both STSM (Figure S7) and PDM (Figure S8) estimation.



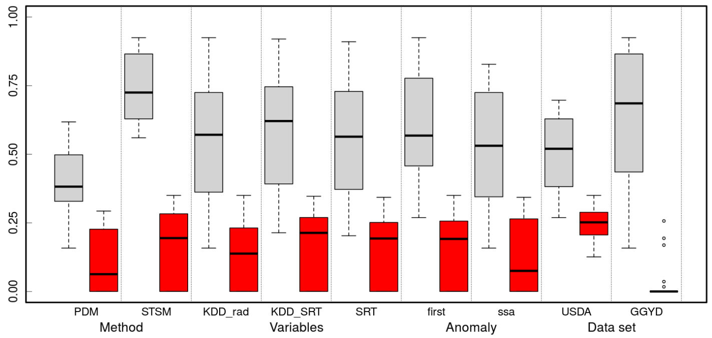
(a) Maize



(b) Soybeans



(c) Spring wheat



(d) Winter wheat

***Figure S6**: Mean model performance (R^2 in gray and R^2_{OI} in red) in the US for different model specifications, split by crops. Abbreviations of the model specifications are provided in the text and Table S1.*

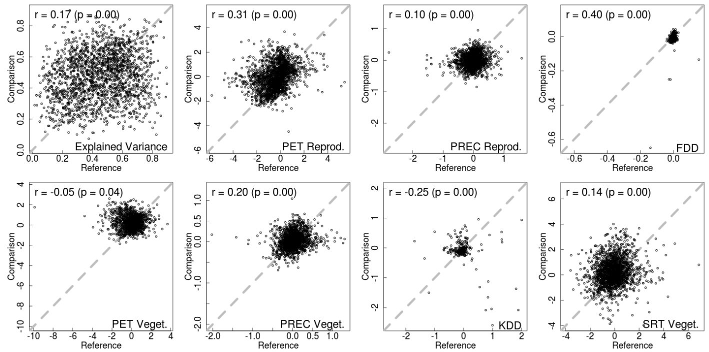


***Figure S7**: Comparison of STSM explained variance and coefficients from USDA ("Reference") and GGYD ("Comparison") maize yield data sets. Each point corresponds to the coefficient estimate for one grid cell. Note that all p-values suggest significance, despite the visual impression of practically no correlation. This significance is owed to the rather high number of data points (1,894), which lets even subtle correlations appear significant.*

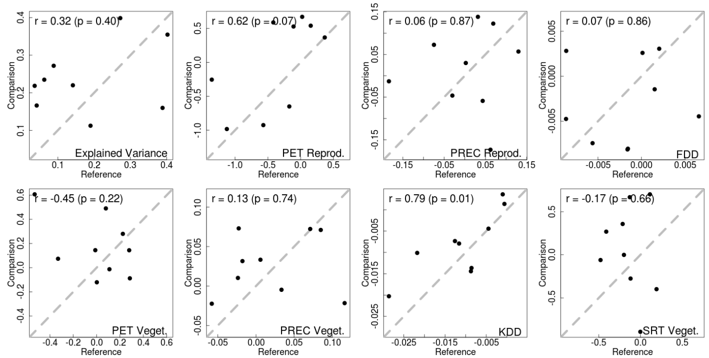
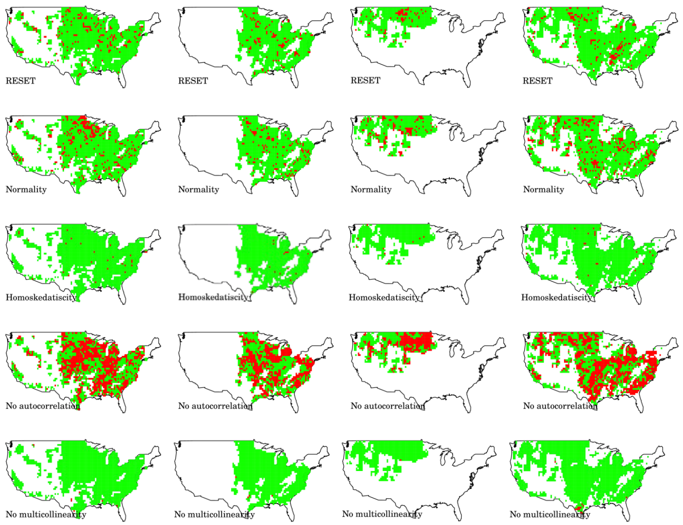


***Figure S8**: Comparison of PDM coefficients from USDA ("Reference") and GGYD ("Comparison") maize yield data sets. Each point corresponds to the coefficient estimate for one aggregation region.*

4. Statistical test results

The results of the statistical tests to ensure model validity are displayed in Figure S9. The RESET test showed that the large majority of grid cells for all four crops were not misspecified, i.e. no quadratic terms were missing. Residuals were normally distributed in most grid cells (Shapiro-Wilk test) and the yield time series were mostly homoscedastic (Breusch-Pagan test). Autocorrelation, however, occurred in a substantial fraction of the grid cells for all crops (Breusch-Godfrey test). This autocorrelation is due to the first difference method and an autocorrelation already in absolute yields (in 55%, 32%, 31% and 37% of grid cells for maize, soybeans, spring and winter wheat, respectively). The LM test for spatial heterogeneity showed, for all crops and all climate regions, that a panel model approach is appropriate (p values < 0.05; no map provided). The condition index test for multicollinearity following Belsley *et al.* (1980) showed values above 10 in only 25 out of 5,976 total grid cells (0.4%) for all crops, and all values are below 17. Since only values above 30 would hint to multicollinearity problems we conclude that this is not a problem.
Thus, with the exception of autocorrelation no test hints to systematic problems for any of the crops.



(a) Maize **(b)** Soybeans **(c)** Spring wheat **(c)** Winter wheat

Figure S9*: Statistical test results for the US. Columns are crops and rows are the different tests. Green indicates a "successful" test, i.e. no problem, while red indicates a rejection of the respective H_0 of no misspecification/autocorrelation/heteroskedasticity/un-normality. For the condition index test of multicollinearity grid cells are marked in red if there is any variable with a condition index larger than 10.*

5. Combined evaluation of observed yield variability and explained variance

The model explanatory power varies to some extent with the observed yield variability. Yield variability here is measured as coefficient of variation (CV), defined as standard deviation over mean. There are four different combinations: whether the model explains more than 45% of the variation or not, and whether yield variability is substantial (CV >= 0.15) or not. We used the values of 45% and 0.15 to conform with a previous study by Ray *et al.* (2015). A combined analysis of these four cases is shown in Figure S10. Regions in green are well explained by the model, with either substantial yield variability (dark green) or not (light green). Regions in blue have low yield variability and this is only less than 45% explained by the model. Regions in red have substantial observed yield variation but the model is not able to capture it. Regions left blank have no harvested area for the respective crop.
The fractions of grid cells with substantial variation but low explanatory power of the statistical model (red pixels) are 23%, 23%, 44% and 36% for maize, soybeans, spring wheat and winter wheat, respectively (Table S2).

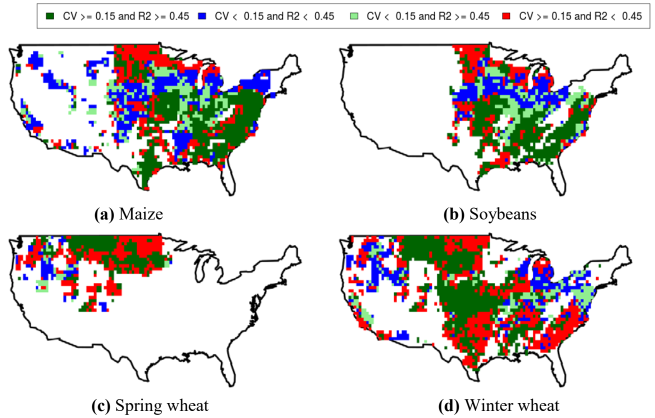


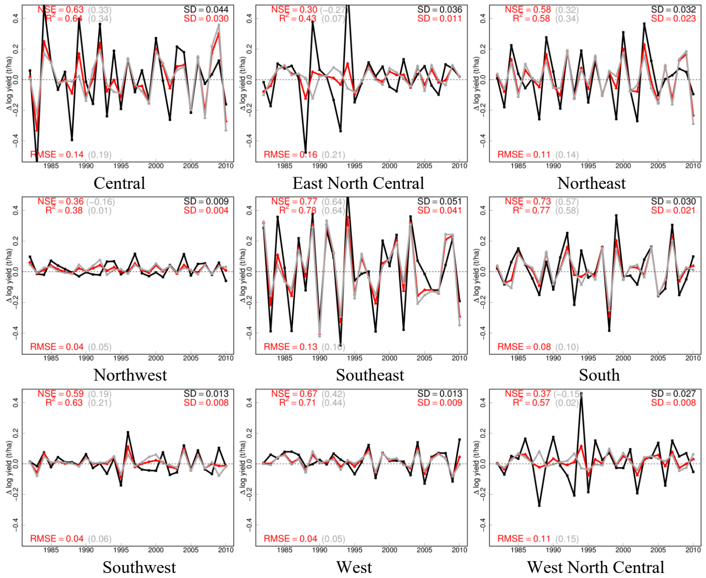
Figure S10*: Combined analysis of model explanatory power vs. yield variation, for USDA maize (panel a), soybeans (b), spring wheat (c) and winter wheat (d).*

Table S2: *Fraction of grid cells (of those where the respective crop is harvested) in different explanation categories (low* R^2*: < 0.45; low* R^2_{O1}*: < 0.25; low CV: < 0.15). Numbers in brackets denote analogue fractions for* R^2_{O1}*. Row sums below or above 100% are due to rounding.*

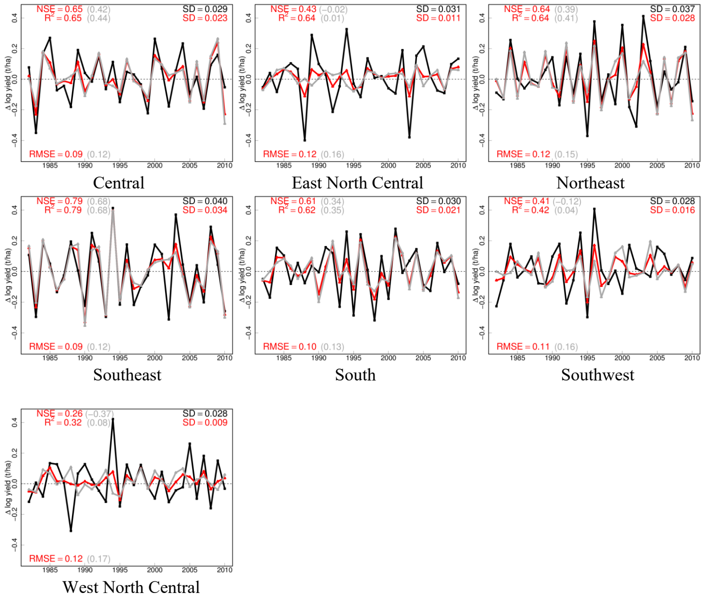
Crop	**Yield data**	**Low CV, low R^2 (R^2_{O1})**	**Low CV, high R^2 (R^2_{O1})**	**High CV, low R^2 (R^2_{O1})**	**High CV, high R^2 (R^2_{O1})**	**Number of grid cells**
Maize	USDA	27 % (33 %)	15 % (9 %)	23 % (35 %)	36 % (23 %)	1,912
Soybeans		20 % (26 %)	17 % (11 %)	23 % (36 %)	40 % (27 %)	1,307
Spring wheat		11 % (14 %)	7 % (4 %)	44 % (64 %)	39 % (19 %)	725
Winter wheat		17 % (20 %)	10 % (6 %)	36 % (50 %)	38 % (24 %)	2,032
Maize	GGYD	40 % (68 %)	48 % (20 %)	4% (8%)	9 % (5 %)	2,021
Soybeans		64 % (84 %)	28 % (9 %)	3 % (6 %)	4 % (1 %)	1,400
Spring wheat		3 % (4 %)	1% (0 %)	42% (65%)	54 % (31 %)	595
Winter wheat		57 % (61 %)	11 % (8 %)	24 % (29 %)	8 % (3 %)	2,036

6. Time series for US regions

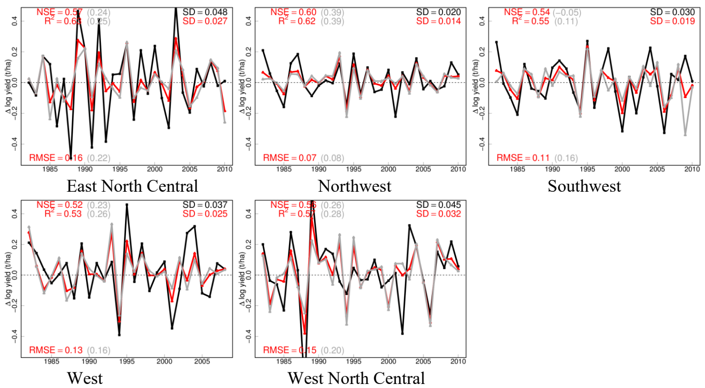
Yield anomaly time series for the nine US climate regions are shown in Figure S11.



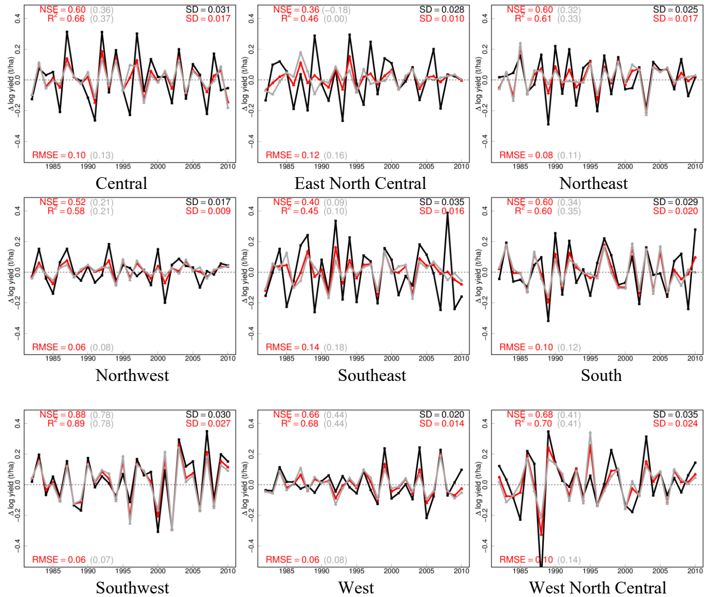
(a) Maize



(b) Soybeans



(c) Spring wheat



(d) Winter wheat

Figure S11*: Yield anomaly time series for the nine US climate regions. Large panels are maize (a), soybeans (b), spring wheat (c) and winter wheat (d). Soybeans and spring wheat are not grown in all regions. Black lines are observed USDA yields, red lines are statistically estimated yields and grey lines are out-of-sample predicted yields. Performance measures printed in red refer to the full model, while grey numbers refer to the out-of-sample estimations.*

7. Model performance for main producers

The list of main producers and the associated three-letter codes are provided in Table S3. Countries can be main producers for several crops, leading to 33 unique countries. Correlations between aggregated GGYD and FAO yields are shown in Figure S12. Yield anomaly time series for the three best reproduced main producers, selected by their R^2_{O1} value, for each crop are shown in Figure S13. For maize and soybeans the time series for the US (which ranks among the top three) is not shown again (see Figure 2 of the main paper) such that we resorted to the next ranks. The number of PDM models estimated within each country depends on its size and the availability of GGYD yield data. Subnational zones are defined by administrative boundaries (GADM1; http://gadm.org/). The only exceptions are Russia, which is represented by the three major agricultural areas around the Caspian and Black Sea, and the USA, which is split into the nine climatic zones as defined in Figure S1.

Table S3*: Main producers for each crop, sorted by descending total production. Main producers are all countries that together produce more than 90% of world production between 2000 and 2011 according to FAO. The number of subnational regions for PDM estimation, if larger than 1, is indicated in brackets behind the country name.*

Maize (24 countries)		Soybeans (5)		Spring wheat (15)		Winter wheat (24)	
Country	**Code**	**Country**	**Code**	**Country**	**Code**	**Country**	**Code**
USA	USA (9)	USA	USA (9)	China	CHN (12)	China	CHN (21)
China	CHN (27)	Brazil	BRA (18)	USA	USA (5)	India	IND (25)
Brazil	BRA (18)	Argentina	ARG (19)	France	FRA (2)	USA	USA (9)
Mexico	MEX (30)	China	CHN (27)	Canada	CAN (5)	France	FRA (21)
Argentina	ARG (19)	India	IND (20)	Australia	AUS (5)	Canada	CAN (7)
India	IND (20)			Turkey	TUR	Germany	DEU (13)
France	FRA (22)			Iran	IRN	Pakistan	PAK
Indonesia	IDN			Poland	POL	Turkey	TUR
South Africa	ZAF			Italy	ITA (19)	Great Britain	GBR
Italy	ITA (19)			Romania	ROU	Argentina	ARG (20)
Canada	CAN (5)			Hungary	HUN	Iran	IRN
Romania	ROU			Syria	SYR	Poland	POL
Hungary	HUN			Russia	RUS (2)	Egypt	EGY
Egypt	EGY			Ukraine	UKR	Italy	ITA (19)
Nigeria	NGA			Kazakhstan	KAZ	Spain	ESP
Philippines	PHL					Romania	ROU
Thailand	THA					Denmark	DNK
Germany	DEU (3)					Brazil	BRA (10)
Spain	ESP					Hungary	HUN
Tanzania	TZA					Syria	SYR
Vietnam	VNM					Morocco	MAR
Ukraine	UKR					Russia	RUS (3)
Russia	RUS (3)					Ukraine	UKR
Kazakhstan	KAZ					Kazakhstan	KAZ

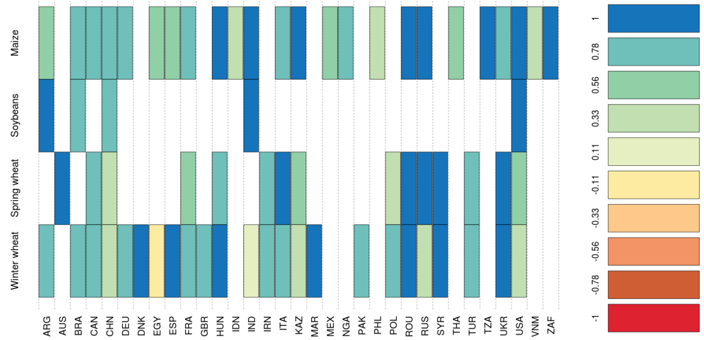
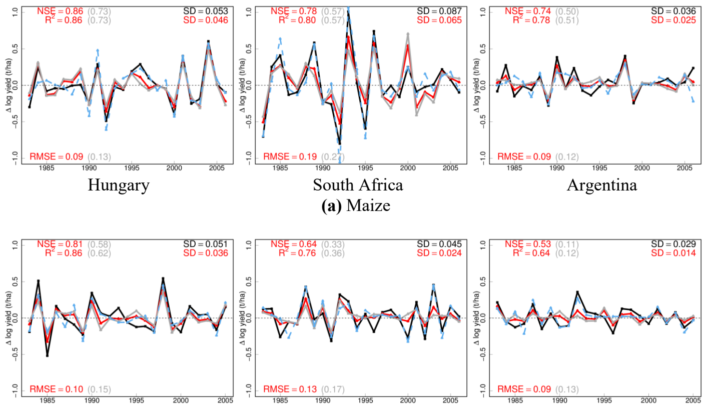


Figure S12*: Correlation (Pearson's r) between nationally aggregated GGYD and FAO national yield anomalies for main producers considered in this study. Yield anomalies were calculated as first differences for both data sets. The MIRCA2000 (Portmann et al., 2010) land-use weighting was applied for aggregation. Applying the M3-Crops harvested areas (Monfreda et al., 2008), which were used for the GGYD construction (Iizumi et al., 2013), instead of MIRCA2000 leads to the same results.*

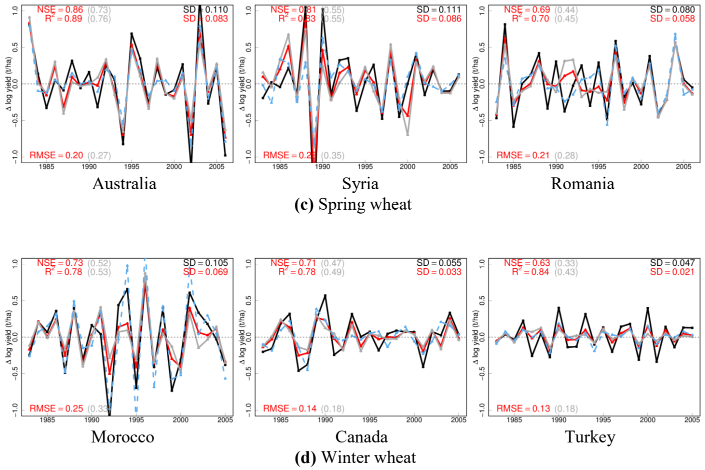


Hungary South Africa Argentina

(a) Maize

Argentina India Brazil

(b) Soybeans



Australia Syria Romania

(c) Spring wheat

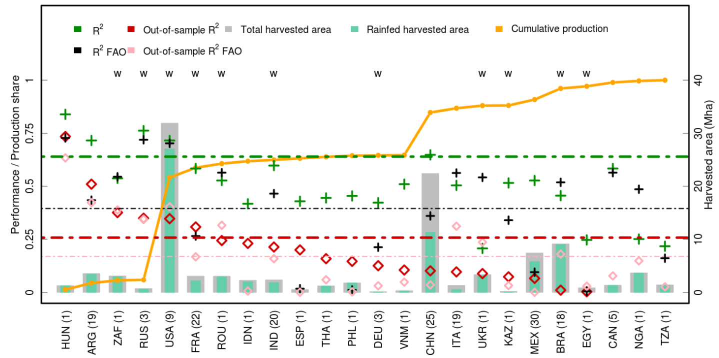
Morocco Canada Turkey

(d) Winter wheat

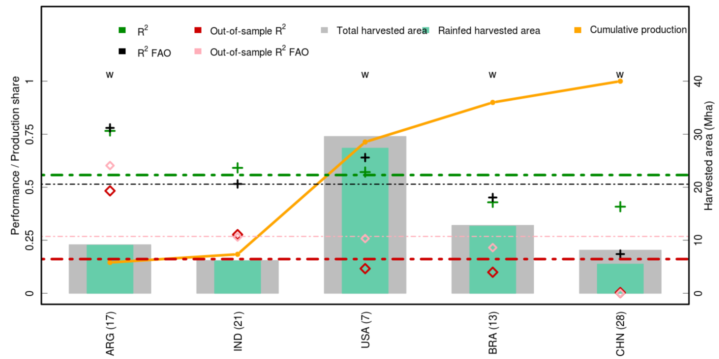
Figure S13*: Yield anomaly time series of selected main producers for maize (a), soybeans (b), spring wheat (c) and winter wheat (d). The three best-performing countries are shown for each crop (excluding the USA).*

8. Results for main producers with PDM estimation

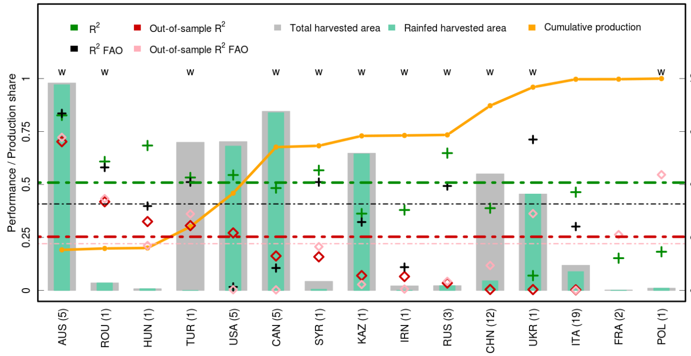
Country performances for PDM estimation with GGYD yield data are shown in Figure S14. The cumulative production share of countries with an R^2_{O1} of at least 25% is 59%, 18%, 46% and 1% for maize, soybeans, spring and winter wheat, respectively. Using the M3-Crops land-use data instead of MIRCA2000 does not change results (data not shown).
Performance measures differ between FAO and aggregated GGYD yield anomalies (black and green crosses for R^2, or orange and red diamonds for R^2_{O1}). This is expectable since FAO yields were not used for model building and therefore represent a cross-prediction evaluation. The average absolute differences are 19, 8, 21, 23 percentage points for maize, soybeans, spring and winter wheat R^2 values, respectively. For R^2_{O1} these differences are 10, 8, 10 and 7 percentage points.



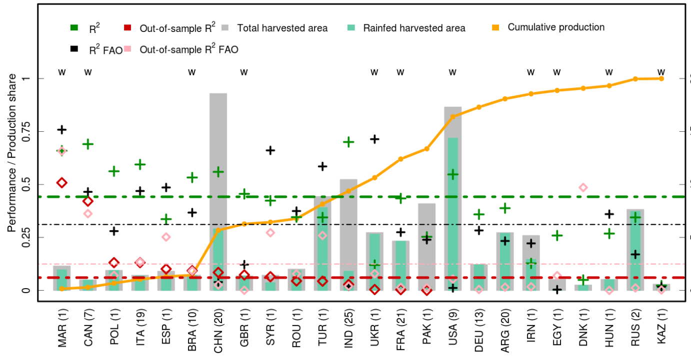
(a) Maize



(b) Soybeans



(c) Spring wheat



(d) Winter wheat

***Figure S14**: Model performances in main producers with PDM estimation. Panels are maize (a), soybeans (b), spring wheat (c) and winter wheat (d). Country order is according to descending R^2_{OI}. Colors and lines are as in Figure 6 of the main paper, with two additional entries: black crosses indicate the R^2 between modeled and FAO yield anomalies, and pink diamonds indicate the FAO-R^2_{OI}, i.e. between out-of-sample predicted and FAO yield anomalies. The number of PDM models estimated per country is indicated in brackets after the country name.*

9. Model performance differences between official yield statistics and GGYD data

The quality of the yield data used for training and evaluating the model is decisive. When using reported yield statistics the out-of-sample performance increases for several countries which otherwise achieve only low performance with the GGYD yield data set (Table S4). In some cases, R^2_{O1} is larger for GGYD than the official data set. This happens only, but not necessarily, if the R^2 from GGYD yields is high (>0.85) and higher than the R^2 from official survey data. For soybeans in Brazil the model trained on GGYD yields shows a better performance than with official yield statistics. Possible reasons are a low matching quality between grid cells and Brazilian provinces (which tend to be smaller than one grid cell), or a general inaptitude of the model for (Brazilian) soybean conditions. This will have to be investigated further.
Note that Burkina Faso is not a main producer, but subnational crop yield data were available to the authors. All comparisons are based on unweighted aggregation.

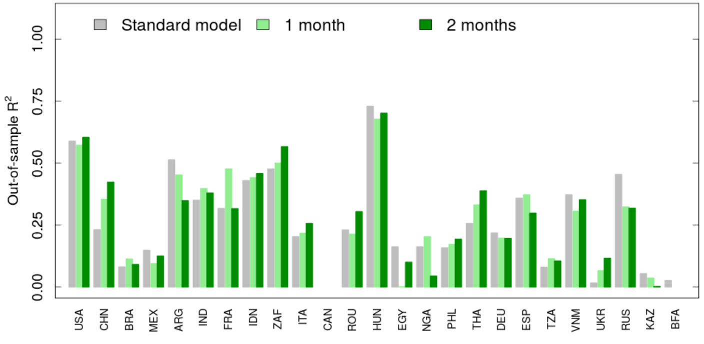
***Table S4**: Different performance of the model when using yield data from statistical offices ("Official") rather than the GGYD data set. R^2_{OI} values which increase by more than 0.1 with official yield statistics are marked in bold.*

Country	Crop	R^2 GGYD	R^2 Official	R^2_{O1} GGYD	R^2_{O1} Official	Data source
USA	Maize	0.92	0.81	0.59	0.55	USDA
	Soybeans	0.77	0.69	0.10	**0.45**	
	Spring wheat	0.73	0.63	0.32	0.34	
	Winter wheat	0.92	0.62	0.04	**0.28**	
Germany	Maize	0.62	0.69	0.22	**0.35**[a]	German statistical offices
	Winter wheat	0.44	0.66	n.a. (r < 0)	**0.20**[a]	
Russia	Maize	0.87	0.84	0.45	0.14	Russian statistical office
	Spring wheat	0.67	0.86	0.01	**0.49**	
	Winter wheat	0.59	0.88	n.a. (r < 0)	**0.34**	
Tanzania	Maize	0.68	0.78	0.08	0.16	Tanzanian statistical office
Australia	Spring wheat	0.89	0.85	0.74	0.66	Australian statistical office
Brazil	Maize	0.83	0.89	0.08	**0.73**	Brazilian statistical office
	Soybeans	0.64	0.41	0.12	n.a. (r < 0)	
	Winter wheat	0.71	0.76	0.13	0.15	
Burkina Faso	Maize	0.59	0.71	0.03	**0.43**	Burkina Faso statistical office

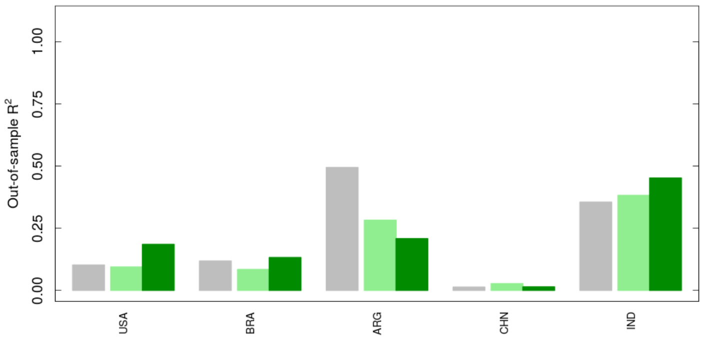
[a] *Note that one-out-of-sample performances for Germany are higher (0.50 for silage maize and 0.61 for winter wheat) in Gornott and Wechsung (2016) where the model is slightly different and uses different weather data.*

10. Forecasting capacity of the model for all main producers

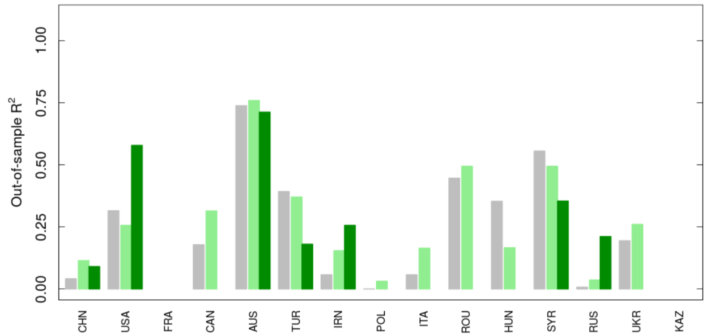
The forecasting capacity of the model, measured by one-out-of-sample R^2_{O1} for prediction with a reduced growing season, is shown in Figure S15. The share of cumulative production within the main producers that can be predicted with at least 25% accuracy one month before harvest is 82%, 18%, 77% and 11% for maize, soybeans, spring and winter wheat, respectively, and with 50% these are 51%, 0%, 19% and 1%. Two months before harvest the production shares with prediction capacity above 25% are 86%, 4%, 36% and 18% for maize, soybeans, spring and winter wheat, respectively, and with 50% these are 51%, 0%, 35% and 1%.



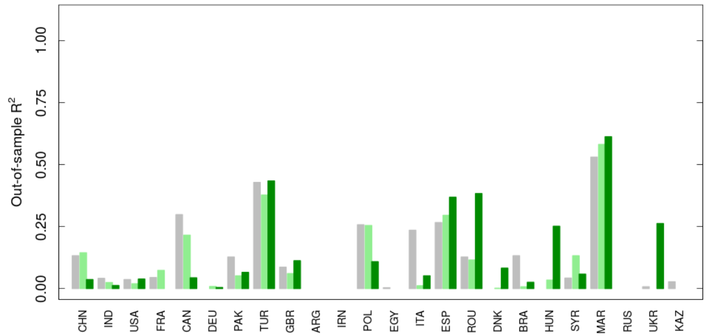
(a) Maize



(b) Soybeans



(c) Spring wheat



(d) Winter wheat

***Figure S15**: Forecasting capacity of the model for all main producers, with GGYD yields. Countries are ordered according to descending total production. Gray bars are the standard model with full growing season used for training and prediction. Green and black bars show performance when withholding one or two months, respectively, for training the model and predicting yield anomalies out of sample. Note that in some cases no performance data are present, for either of two reasons: the reduction of the growing season did not allow for calculating any regression, or the correlation between observed and predicted anomalies is negative and thus its squared value would be misleading.*

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6 Synthesis and outlook

6.1 Different improvements of crop models to better assess agricultural production have been presented

In the preceding four chapters of this thesis it has been researched how to improve crop models for a more precise quantification of weather influences on yield variability. The results are shortly revised here and put into the context of food security.

In the second chapter, a novel method for literature mining and systematic knowledge structuring has been applied to comprehensively review the drivers and mechanisms of yield variability from a large number of scientific references. There are three main results of the analysis. First, a comprehensive network of interactions between growing conditions, plant physiological processes and crop yield is constructed. The network allows for a visual exploration of interactions and, together with the annotated references, for a quick start into a deeper literature research. This visual exploration can support the implementation of selected processes into crop models. Second, a detailed list of amendment suggestions for crop models is derived from the interaction network. Third, the study introduces a new approach for reviewing experiment-based knowledge on plant processes at different scales and levels of complexity. This method is scalable, can be generalized to different topics and has potential for automatization, which can fasten the tedious process of knowledge mining and structuring. There is no direct connection of this study to food security, but the manifold interactions extracted from the literature reflect the diversity of influences on agricultural performance and have been useful in delineating the research questions of the other chapters.

In the third chapter, a newly implemented ozone-damage module in the global vegetation model LPJmL has been used to simulate historical wheat and soybean crop losses from O_3 pollution. Results indicate that ozone is a major problem for crop production in several countries with losses around 8% for wheat in Europe and occasional losses up to 50% in South Asian wheat. Simulated effects have been shown to compare well with previous studies when run under similar conditions, but also reveal differences if other environmental factors modify the damage potential of ozone. This highlights that co-factors of ozone damage, namely water status, temperature and CO_2, need to be considered for robust loss estimations. The presented study is the first global assessment of historical yield losses from ozone including these co-factors. Yield losses from ozone pollution reduce food availability and thus unnecessarily endanger food security since effective counter-measures against ozone are well known (Shindell et al., 2011). The assessment in chapter three indicates that particularly regions in South Asia would profit from a mitigation of ozone pollution. Such mitigation would also be beneficial for human health, which is negatively affected by ozone pollution, too (Rao et al., 2016; Shindell et al., 2011).

In the fourth chapter, nine process-based crop models have been evaluated with respect to their representation of high-temperature effects on maize, soybean and wheat crop yields in the US. This evaluation has revealed three key insights. First, process-based crop models are able to reproduce effects of high temperatures above 30°C on crops. This is highly relevant when using crop model outputs for economic projections, which may put emphasis on non-linear production losses. Second, the main mechanism behind the yield loss is identified as water deficit rather than direct plant damages - at least until a threshold of approx. 36°C, where sufficient observations are available. This was previously unknown on the large geographic scale considered here and justifies irrigation as an appropriate counter measure where water is available. Third, contrary to long-held assumptions, the study hypothesizes that elevated CO_2 cannot prevent yield losses due to high temperature stress in the future. This hypothesis may stimulate field experiments to test its validity. Recent results already point towards validity, at least for grassland (Obermeier et al., 2017). Furthermore, the study confirms that model ensembles are more reliable than single models, which are not able to reproduce observed crop responses in some cases. The individual temperature-response curve of each model may portend to specific improvement options for models. In the context of food security, this study underlines the risks that high temperatures pose for crop production and thus food availability and stability already today and particularly in the future.

In the fifth chapter, an existing statistical crop model has been extended by extreme temperature penalties and applied to three tasks. First, the model is extensively evaluated in the US and indicates that weather influences on crops are highly regionalized and dependent on crop phenology. These results conform with expectations and highlight both validity and generalizability of the model. Second, the global share of maize, soybean and wheat yield variability attributable to weather variability is estimated around 40%, though the exact number depends on crop, measurement variable for attribution and regional yield data quality. The varying quality of the utilized yield data, due to their derivation from remote sensing, makes estimations more difficult. In the study it is shown that a high quality of the yield data base, used for developing and validating the model, is an indispensable component of assessing environmental influences on agricultural production. Furthermore, the substantial share of weather influence on crop production shows risks for global food production if weather patterns change under global warming, in particular if there is an increase of heat days. Third, the capacity of the model for near-term forecasts of yields within the growing season is measured. The results of this exercise illustrate its application potential, with robust results that allow for a deepening of this approach. Such near-term forecasts can help to mitigate or avoid food security crises by supporting the preparation of adequate counter measures.

6.2 Open questions for future food security remain

Three paths for further studies of climate change effects on food security are accentuated, based on findings in the previous chapters. First, the effect of ozone on crop yields in the future is of relevance for availability and stability of food supplies. To this end, existing uncertainties of the module introduced in chapter three should be reduced and its spectrum of crops be extended. Then LPJmL with the O_3 module can be used for such an assessment. A combined assessment of impacts on agricultural production and human health from ozone would be of interest, too. Second, the effect of extreme heat above approximately 36°C - where there are only few observations available currently - needs to be studied in experiments and then implemented in crop models. This would allow for more realistic assessments of crop losses under very adverse conditions, which are more likely with unabated global warming. Third, the forecasting of yields within the growing season is of eminent importance for agricultural and political management. The basic approach portrayed in chapter five can be enhanced for practical applicability, for example by integrating remote sensing data and near-term weather forecasts into the model.

This thesis addresses two central dimensions of food security: the availability and stability of agricultural production. The availability of food from other sources other than agriculture, the stability of prices and incomes and the two dimensions of access and utilization also merit attention (Figure 1.1). Yet their assessment requires integration of biophysical and socio-economic models, which goes beyond the scope of this thesis. Also within the availability and stability dimensions, other influences on crop yields like flooding, storms or pests and diseases have not been treated here. To reduce uncertainties in projections of climate change impacts on future yields, however, these influences are certainly of relevance. Additionally, nutrition security, which goes beyond only sufficient calories by including indicators like the content of protein and other nutrients in food, has not been studied. Yet this is a necessary prerequisite for food security (Gustafson et al., 2015) and, consequently, the inclusion of grain quality in crop models has recently earned more attention (Nuttall et al., 2017).

In this thesis it has been exemplified that the manifold influences of weather may endanger food security, and particularly so under an unabated change of climate. Therefore mitigation of climate change is the best option if severe impacts on crop production should be avoided, since even with a global warming limited to 1.5 or 2°C - as the Paris Agreement demands - impacts on crops can be expected (Schleussner et al., 2016b). Complementary to climate change mitigation, there are numerous avenues for the improvement of food provision, as the suggestions provided by the sustainable intensification and climate-smart agriculture debates prove (Godfray et al., 2010b; Lipper et al., 2014). All these measures could contribute to making agriculture and food security a full global success story.

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Selbständigkeitserklärung

Ich erkläre, dass ich die Dissertation selbständig und nur unter Verwendung der von mir gemäß §8 der Promotionsordnung der Landwirtschaftlich-Gärtnerischen Fakultät, veröffentlicht im Amtlichen Mitteilungsblatt der Humboldt-Universität zu Berlin Nr. 12/2014 am 31.03.2014, angegebenen Mittel angefertigt habe.

Paris, den ____________________ ________________________________

Datum Unterschrift